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Particles and biomembranes: a variational PDE approach

by

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Thesis

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To Mum, Dad, Matt and all of my family who have supported me and helped me to get to this point, thank you all. To Amy, thank you for everything, I love you.

Declarations

This thesis is submitted to the University of Warwick in support of my application for the degree of Doctor of Philosophy. It has been composed by myself and has not been submitted in any previous application for any degree. The work presented was carried out by the author except for Appendix B which is collaborative work with Carsten Gräser of Freie Universität, Berlin.

Parts of this thesis have been published by the author, Chapter 2, Chapter 3, Appendix A and Appendix C appear in a paper co-authored with Charlie Elliott, Carsten Gräser, Ralf Kornhuber and Maren-Wanda Wolf, *A Variational Approach to Particles in Lipid Membranes*, published in Archive for Rational Mechanics and Analysis [31]. Chapter 4 and Appendix D form the basis of a paper co-authored with Charlie Elliott and Hans Fritz, *Small deformations of Helfrich energy minimising surfaces with applications to biomembranes*, which has been submitted for publication.

Abstract

We examine mathematical models for small deformations of membranes. First we review physically well established models, posed in the Monge gauge, from a mathematical perspective. We produce a variational framework in which well posedness can be studied and finite element methods applied. The methods are used to investigate the effects of point forces, point displacement constraints and point curvature constraints. Such models are suitable for the study of deformations induced by filaments contained in the cell cytoskeleton and by embedded protein inclusions. In particular we study the membrane mediated interactions between filaments and also between inclusions.

We then introduce a new linearised model which describes small deformations of closed surfaces that are minimisers of Helfrich-type energies. The deformed surface is described as a graph over the Helfrich minimising undeformed surface. This is the natural generalisation of the Monge gauge to initially curved surfaces. We focus on a Willmore energy which gives rise to spheres and a family of tori as undeformed surfaces and also introduce surface tension on a sphere. Again we study deformations induced by filaments. A variational formulation is produced which is similar to the Monge gauge case and we formulate a numerical method to study membrane mediated interactions.

Finally we introduce an abstract splitting method which allows a high order PDE to be solved by an equivalent system of lower order equations. We give conditions which ensure well posedness of the system and produce a finite element method whose solution converges to the solution of the full system. The theory is applied to show convergence for the numerical methods used for the surface deformations model. We provide examples which show the theoretical error estimates are achieved.

Chapter 1

Introduction

1.1 Biological membranes and deformations

Biological membranes (biomembranes) are found in every living cell. They form the barrier between the cell and its surroundings and also between cell organelles and the cytoplasm in eukaryotic cells. This allows the cell to control levels of various substances within it, permitting a variety of chemical reactions both on the membrane surface and within membrane enclosed regions.

The membrane consists of a phospholipid bilayer with embedded and attached proteins. The bilayer is made of phospholipid molecules which are composed of a phosphate group head and a lipid chain tail. The head is hydrophilic whilst the tail is hydrophobic, hence when placed in water they form structures where the heads point outwards and the tails inwards. There are a number of such structures, here we are interested in the bilayer sheet which is the one that forms cell membranes. In this formation the heads form two distinct layers with the tails sandwiched between them. A portion of this structure is shown in Figure 1.1 which is taken from [56] and appears in [31]. The bilayer sheet has elastic properties which allow it to be

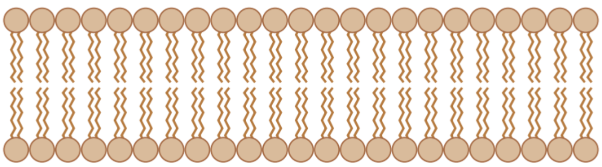

Figure 1.1: Phospholipid bilayer sheet

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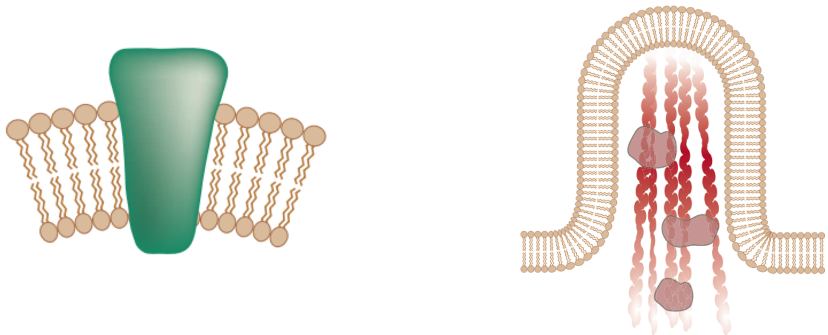
deformed and interact with both the embedded and attached proteins as well as other exterior stimuli. Modelling these interactions and deformations is the main theme of this thesis.

Due to the great variety of cells and their functions there are many mechanisms for membrane deformation. However each of these mechanisms falls within one of five broader categories presented in [56]. These categories are: inhomogeneous lipid composition, influence of embedded or transmembrane proteins, interactions with the cytoskeleton, scaffolding and helix insertion. Here we will focus on the influence of embedded or transmembrane proteins and interactions with the cytoskeleton, though the other types of deformation are not beyond the scope of the models we will introduce. These two types of deformation are illustrated in Figure 1.2 which is taken from [56] and appears in [31].



(a) transmembrane protein (b) filaments anchored in the cytoskeleton

Figure 1.2: Protein-induced membrane deformation

Embedded or transmembrane proteins affect the membrane as it locally conforms to the shape of the protein. For example a conical protein will induce a local curvature in the membrane. This has been observed experimentally for the nicotinic acetylcholine receptor in [76].

The cytoskeleton interacts with the membrane via actin filaments. These are thin filaments which are anchored to the cytoskeleton. Under certain conditions the filaments undergo polymerisation which causes a protrusive force to be applied to the membrane [55]. We will now move to discussing how these biological phenomena are modelled mathematically. For a more complete description of the biological processes see [56] and the references therein.

1.2 Mathematical model

A key question in modelling the deformations of biomembranes is how to account for the various length scales involved. Cell membranes have a typical thickness $7.5 - 10nm$ [41] whilst cells can reach diameters up to $10 - 100\mu m$ [54], causing a difference of four orders of magnitude in two of the length scales of interest. Membrane proteins typically have diameters comparable to the thickness of the membrane and can interact via the membrane over length scales $6 - 100nm$ [33], this is a third length scale of interest which sits between the two discussed above. We can group particular models for membrane deformation by how these relevant length scales are treated.

Coarse grained molecular models are formed by representing the phospholipid and protein molecules as short chains of beads with appropriate pairwise interaction potentials. The behaviour of the system is studied as the membrane evolves from some initial state via the pairwise interactions. This method is used to study the interactions of membrane proteins with a biomembrane in [67, 69, 73]. Such models are highly detailed, accounting for many of the physical properties of the individual molecules which make up the membrane. As such they provide a precise description of interactions between proteins and the membrane up to a very short length scale, this is important in studying cluster formation for example. The level of detail comes at a relatively high computational cost however. To produce these molecular dynamics simulations requires repeatedly solving a very high dimensional system of equations. A natural way to attempt to reduce this computational cost is to look for more macroscopic models. That is we look for models which do not necessarily account for the behaviour of every single molecule but still capture features of interest, such as the way membrane proteins interact with each other.

The most macroscopic models are referred to as continuum models and are based around the Canham-Helfrich model of lipid membranes [39, 40]. Here the membrane is taken to be a single elastic sheet whose deformation is governed by the Canham-Helfrich bending energy. This energy is closely related to the Willmore energy [81] which appears in differential geometry. The lipid and protein components of the membrane are modelled by concentrations which affect the bending rigidity and spontaneous curvature of the membrane. Minimising the resulting energy determines the equilibrium shape of the membrane. Such a minimisation problem can be rewritten as a partial differential equation and coupled to equations governing the evolution of lipids of proteins on the membrane, producing a more detailed model. Such an approach is taken in [28, 30] which reproduce typical equilibrium shapes of vesicles such as dumbbells, discocytes and starfishes.

Hybrid models sit in between these two scales. The intention is to produce models that capture interactions between individual proteins, which continuum models are unable to do, whilst maintaining a lower computational cost than molecular dynamics based models. They are thus well suited to studying behaviour at moderate length scales. The approach taken is to treat the membrane as continuous, obeying the Canham-Helfrich energy, but the proteins as discrete. The proteins are coupled to the membrane either by some boundary conditions or by adding coupling terms to the membrane energy functional. Hybrid models have become a well established part of the theoretical physics literature, see for example [23, 24, 36, 39, 43, 48, 53, 61, 63, 65, 78, 83, 84]. Similarly to continuum models the overall aim of hybrid models is to produce partial differential equations which describe membrane behaviour, here the focus is on membrane-mediated interactions between individual proteins. As the large number of references suggests, there are a tremendous amount of these hybrid models. In this thesis we aim to introduce a general mathematical framework into which these models can be placed, we will study a few in more detail but in principle the techniques we use can be adapted to any of the hybrid models in the references above and a great many more that exist in the literature.

In creating hybrid models one treats the proteins either as points as in [4, 23, 24, 48, 53, 60, 61, 80] or as having some finite size [36, 39, 43, 48, 59, 63, 70, 78]. Each method has its own advantages. In general the finite size particle models produce lower order partial differential equations but on more complex domains with more complex boundary conditions. The point models require more regularity to be well posed so produce higher order equations but it is simpler to move particles around and explore the membrane mediated interactions. In this thesis we will focus on point models, to see how this compares with the finite sized particles approach see [31].

1.3 Point models

Point models can be used for a number of forms of membrane deformation, here we focus on curvature inducing embedded proteins and interactions with the cytoskeleton. Curvature inducing proteins are modelled as points frequently in the physics literature, for example in [24, 53]. However the underlying models studied in these two papers, amongst others, are not well posed from a mathematical point of view. They study a Canham-Helfrich energy for u, the displacement of the membrane from a flat configuration occupying a domain $\Omega \subset \mathbb{R}^2$, this takes of the form

$$E = \int_\Omega (\Delta u)^2.$$

Coupled to this energy are constraints or forces which act at a single point. However, these constraints or forces require the point evaluation of a second derivative of u. Mathematically this creates a problem as the natural space in which to pose an energy minimisation problem based on E is $H^2(\Omega)$, that is the space of functions with square integrable weak derivatives up to second order. To make sense of the forcing or constraints however we need u to be C^2, at least at the locations of the particles, this is much more regularity than a general $H^2(\Omega)$ function possesses. The issue is avoided in [24, 53] by using expansions with a suitable truncation. We will consider a different approach, used in [4], of taking a higher order elastic Hamiltonian. This allows the resulting problem to be well posed mathematically.

We will also consider the interaction of the cytoskeleton with the cell membrane. The first interaction we consider is the protrusive force applied to the membrane by actin filaments. A detailed physical model for this interaction is given in [62]. Such forces have also been modelled in a continuum setting in [37, 77], where the effect of the forces is coupled to the diffusion of activator proteins within the membrane. We aim to produce a hybrid model based on assuming the protrusive forces act at single points. The model is similar to the one proposed in [33], taking the general force distribution used there to be a linear combination of point forces. This allows us to explore the membrane mediated interactions between the protrusive forces which are omitted from the continuum model in [37]. We will also consider a simple model for how the cytoskeleton determines the membrane shape. We suppose that the displacement of the membrane is fixed at certain points, corresponding to the action of filaments anchored to the cytoskeleton. This is a much simplified version of the model used in [17] where the force applied by a fluctuating membrane to such a filament is examined.

1.4 Membrane geometry

To date, much of the research into hybrid models has been carried out in the Monge gauge. That is the membrane is assumed to be approximately flat with small deformations occurring in the normal direction. The membrane is thus described as a graph over a two dimensional planar domain. This is not the only circumstance in which the Canham-Helfrich model is valid however. In [40] the model is posed in a more general geometrical setting. The deformations of membranes in more complex geometries has been considered for finite sized particles in [59, 70]. There are also continuum models which couple the Canham-Helfrich energy to surface dynamics to predict equilibrium membrane shapes, see [28, 29, 30]. The geometric partial differential equations which result from these models are coupled nonlinear systems, effectively solving such systems is an active area of mathematical research. Here we work in the spirit of the linearised models produced in the Monge gauge. That is we look to generalise the technique of linearisation for the Canham-Helfrich energy in the Monge gauge to graphs over more general surfaces. Although we will study point models here, the techniques used could be generalised to treat finite sized particles and hence produce a framework into which the models considered in [59, 70] may be placed.

1.5 Mathematical problems

We will begin by studying a model for the interaction of the cytoskeleton with the membrane via point forces. Mathematically, this involves solving a fourth order partial differential equation over a two dimensional planar domain Ω. The PDE results from the minimisation of an energy over the space $H^2(\Omega)$ subject to some appropriate boundary conditions. A typical equation is of the form

$$\Delta^2 u = \delta_X.$$

The right hand side of this equation is a delta function or a linear combination of delta functions, resulting from the point forces applied to the membrane. We also consider a similar minimisation problem involving point constraints which, when approximated via a penalty method, produces a similar PDE. A further minimisation problem where the locations of the forces or constraints may vary along with the shape of the membrane is also studied. This further minimisation is a general exploration of the membrane mediated interactions between individual point forces or point constraints. Much of the physics literature in this area is concerned with calculating explicit interaction laws, we will not do this here. Instead we will present a result about the global behaviour of the system, finding the configuration of particles and membrane which globally minimises the energy.

To examine the point force and point constraint models we numerically solve the resulting PDEs via a finite element method. This and all of the finite element methods used in this thesis have been implemented within the Distributed and Unified Numerics Environment (DUNE) framework [5, 6, 9, 19], see also the web pages [7, 20]. DUNE is a modular toolbox for solving PDEs from which the finite element methods used in this thesis can be readily implemented.

The direct solution of fourth order PDEs requires a finite element method which is suited to H^2 problems. To create a H^2 conforming finite element one must use a relatively large number of degrees of freedom on each element. For example the Hsieh-Clough-Tocher element requires 10 degrees of freedom and the Argyris element 21, see [15]. One could also attempt to use non-conforming finite elements, for example the Morley element [15, 51], these elements use fewer degrees of freedom but present their own challenges, particularly for surface PDEs. Here we will take a different approach and use a splitting method to turn a fourth order PDE into a system of two second order equations which can be solved with much simpler finite elements. Such a technique leads to solving saddle point problems, similar to the one appearing in [16].

We will model the effect of embedded inclusions by point curvature constraints. This is approached in the same manner as for the previous point constraint model but requires a higher order membrane energy. This leads to energy minimisation problems posed over $H^4(\Omega)$ with constraints applied to second derivatives of the displacement u. Using a penalty method one can rewrite the problem as a PDE, taking a form similar to

$$\Delta^4 u = \partial_{x_i x_j} \delta_X.$$

As with the previous PDE, this equation is meant only in the sense of distributions. To solve this equation numerically requires a splitting method, whilst it is possible to construct H^4 conforming and non-conforming finite elements their implementation would be prohibitively difficult. As such we will employ a splitting method which reduces the problem to a system of second order equations.

To produce a linearised Canham-Helfrich model for deformations from more general surfaces we will consider an energy functional which is a small perturbation of the Willmore functional [81]. Under the ansatz that the resulting surface is sufficiently close to a Willmore surface, that is a surface which is a critical point of the Willmore functional, we produce a second order approximation of the energy via a Taylor expansion. In this thesis we consider two such Willmore surfaces, a sphere and a Clifford torus. We then pose point force and point displacement constraint problems for these surfaces in a similar manner as in the Monge gauge. The surfaces present an additional complication however as the bilinear form we use, the second variation of the Willmore functional, has a non-trivial kernel over these surfaces, this is not the case in the Monge gauge. For the sphere the kernel is easily identified, for the Clifford torus this has been done previously in [58]. Having appropriately posed these problems they can be solved numerically using a splitting technique similar to the one used for the planar problems.

Finally we shall present an abstract saddle point problem and related finite element method. This theory can be applied to show the well posedness and convergence of the splitting and finite element methods outlined above. The abstract saddle point problem is similar to one studied in [16] and particularly in the cases studied in [47, 82]. The saddle point problem is a weak formulation of a block matrix problem of the form

$$\begin{pmatrix} A & B \\ B & -C \end{pmatrix} \begin{pmatrix} u \\ w \end{pmatrix} = \begin{pmatrix} F \\ G \end{pmatrix}.$$

In [16, 47, 82] it is assumed that the operator A induces a bilinear form that is either coercive or at least positive semidefinite. Here we relax this assumption, though need to make a stronger assumption on C to accommodate this. The alteration is motivated by the variational problems posed over the torus. The second variation of the Willmore functional is somewhat complex, making it difficult to construct a splitting which produces a saddle point problem where each of A, B and C satisfy the assumptions made in [16].

1.6 Biophysics applications and further work

The problems studied in Chapter 2 are strongly motivated by [33]. There the minimisation of the Canham-Helfrich energy in the Monge gauge is considered when the membrane is subject to some general forcing f. The resulting energy functional is given by

$$F = \int_{\mathbb{R}^2} \frac{\kappa}{2}(\Delta u)^2 + \frac{\sigma}{2}|\nabla u|^2 - fu.$$

Note that the membrane is considered to be infinite, it is described by a graph over the whole of $\mathbb{R}^2$. In Chapter 2 we consider only bounded domains $\Omega \subset \mathbb{R}^2$, the distinction is minor however provided we take a sufficiently large domain.

A formula for the minimising function u is computed in terms of the Green's function for the Laplacian integrated against the forcing f. This formula is used to produce an interaction potential between two protein particles by choosing a specific form for f which depends upon the location of the two particles. The interaction potential is explicitly calculated for a particular case, the interaction of two circularly symmetric inclusions, and approximated for elliptical inclusions with a large separation. It is noted that interaction potential cannot be computed analytically when the inclusions are not circularly symmetric. This issue is a potential application for our work.

Whilst this thesis focuses on a particular form for f, related to point forces applied to the membrane, the analysis and techniques in Chapter 2 may be applied to any $f \in W^{1,q}(\Omega)^*$, for some $2 < q < \infty$. Such a condition permits the study of a broad class of forcing functions f. Then for any two inclusions, provided we can produce a location dependent $f \in W^{1,q}(\Omega)^*$ which describes the force applied to the membrane, we can numerically approximate the solution u via the finite element method introduced in Section 2.4. By moving the locations of the particles, for example by increasing their separation, we can then approximate the interaction potential. If we are simply interested in the qualitative properties of the interactions rather than producing an interaction potential one could move the particles according to a gradient flow. This would provide a simple means to explore the many body system if we had a larger number of particles.

The point curvature constraints problems studied in Chapter 3 are derived from the model introduced in [4]. Here a curvature inducing protein is modelled by applying point constraints to the second derivative of the displacement. Well posedness of the minimisation problems is ensured by studying a higher order bending energy which now also includes the terms

$$\frac{1}{2}\int_{\mathbb{R}^2} (\Delta^2 u)^2 + \kappa_6 |\nabla \Delta u|^2.$$

The interaction potential is approximated for two identical isotropic inclusions, that is inclusions which fix the curvature to be

$$(u_{xx}(X), u_{xy}(X), u_{yy}(X)) = (c, 0, c),$$

for some $c \in \mathbb{R}$. Moreover the dependence of the interaction upon the rigidity of the particle is explored. Each of these results can be reproduced within the framework introduced in Chapter 3 using the finite element method. Furthermore, we could use a gradient flow technique to study the interactions of particles in a many body system and identify equilibrium energy states. Such a many body system is considered in [24], there the equilibrium state is found using a Monte Carlo method to move each individual particle and accept moves which lower the total energy of the system. A gradient flow method would be more efficient for finding equilibrium states since every step lowers the energy of the system.

A further application of this work could be towards the model considered in [70]. Here the membrane is assumed to be a sphere but constrained to take a particular shape in some region, modelling protein scaffolds which locally determine the shape of the membrane. The equilibrium shape of the membrane is then determined by minimising the Willmore energy subject to these constraints. Interaction potentials are then calculated for particular scaffolds. We could put this model in our framework in a number of different ways. For example we could follow a similar procedure to the point constraints problem set up in Chapter 4 except constrain the membrane displacement over a given area rather than at a point to model the scaffolding. This would produce a linearised problem which is a good approximation to the one studied in [70]. We have another option to model this phenomenon however. The numerical results in [70] indicate that the membrane deformation is localised to the vicinity of the protein scaffolds, away from the scaffolds the membrane essentially remains spherical. This indicates a good approximation could be made by using the Monge gauge. To do so we would take a cross section of the sphere at $z = z_0$ such that all of the scaffolds lie within the remaining membrane. The remaining membrane can then be described as a graph and we may apply the theory developed in chapters 2 and 3. In particular we could model the scaffolds by following the procedure in Chapter 2 and constraining membrane displacement over given regions, by making a point approximation as in Chapter 3 or by introducing the constraints as boundary conditions as in [31]. Each of these methods should in theory be more efficient than solving a problem based on the whole surface since the displacement from a sphere is essentially zero away from the inclusions. A comparison of their relative effectiveness compared to performing computations over the whole sphere could prove to be interesting.

1.7 Structure of thesis

In Chapter 2 we introduce the Canham-Helfrich energy and its linearisation in the Monge gauge. This leads to energy minimisation problems which model membranes under the influence of point forces or point displacement constraints. We then present a splitting method and numerical method for the solution of the resulting partial differential equations. We show convergence for the numerical method along with a numerical study of the membrane mediated interactions between point forces and point constraints.

In Chapter 3 we consider an augmented Canham-Helfrich energy and introduce point curvature constraints. This produces a higher order minimisation problem which is equivalent to an eighth order PDE. A splitting method and related finite element method is then produced to explore membrane mediated interactions between the point constraints.

The work in Chapter 4 generalises the linearisation of the Canham-Helfrich energy to initially curved surfaces, namely the sphere and Clifford torus. We also introduce surface tension on the sphere. We then present point forces and point displacement constraints analogously to Chapter 2. Finally, a numerical method based on second order splitting is produced to explore these two problems.

Chapter 5 focusses on an abstract splitting method which is motivated by the problems appearing in Chapter 4. We then formulate an abstract finite element method based upon the splitting and prove convergence. The abstract theory is applied to solve the problems formulated in Chapter 4 and a further model problem.

The material in Appendix A covers some general abstract results related to minimisation problems and penalty methods. This general theory is applied in chapters 2, 3 and 4. Appendix B presents coercivity results for the bilinear operators used in chapters 2 and 3. Appendix C presents regularity results for the PDEs formulated in chapters 2 and 3, these results motivate the choices of spaces used in the second order splitting methods. Finally, Appendix D contains the calculations required to produce the second variation of the Willmore functional which is used in Chapter 4.

Chapter 2

Fourth order problems on a planar membrane

2.1 Canham-Helfrich free energy

As the width of a bilayer ($10^{-9}m$) is much smaller than its lateral extension, it is natural to model the membrane as a smooth, two-dimensional hypersurface $\mathcal{M}$ embedded in the three-dimensional Euclidean space $\mathbb{R}^3$. Note that this simplification neglects transversal stretching and transversal shearing as possible elastic deformations. Since the fluidity of the membrane excludes lateral shearing, the deformations of the membrane are caused by lateral stretching and bending.

The mathematical study of biomembranes principally concerns the minimization of the energy functional describing the energy associated to displacements of $\mathcal{M}$. Fundamental to the macroscopic approach to modelling biomembranes is the Canham-Helfrich (CH) model [13, 34, 40] which is based on the expansion of the bending energy with respect to the principal curvatures up to second order. It describes equilibrium and close-to-equilibrium properties of biological membranes. The fundamental object of the CH model is the elastic bending energy $\mathcal{J}_{CH}$ defined by

$$\mathcal{J}_{CH}(\mathcal{M}) = \int_{\mathcal{M}} \tfrac{1}{2}\kappa(H - c_0)^2 + \kappa_G K \; d\mathcal{H}^2. \tag{2.1}$$

Here H and K stand for mean and Gaussian curvature of the membrane $\mathcal{M} \subset \mathbb{R}^3$ while κ, $\kappa_G > 0$ are the corresponding bending rigidities and $\mathcal{H}^2$ is the 2-dimensional Hausdorff measure. The additional parameter c_0 is called *spontaneous curvature* and accounts for a possible asymmetry between the outer and inner layers in the otherwise flat reference configuration, e.g., due to different lipid compositions in the layers. The related energy

$$\mathcal{J}_{CHS}(\mathcal{M}) = \int_{\mathcal{M}} \tfrac{1}{2}\kappa(H - c_0)^2 + \kappa_G K + \sigma \, d\mathcal{H}^2 \tag{2.2}$$

supplements the bending energy with a surface energy $\int_{\mathcal{M}} \sigma \, d\mathcal{H}^2$ that is associated with membrane tension $\sigma \geq 0$. Here, the surface energy penalises area change and thus accounts for the incompressibility constraint of the fluid membrane in the lateral direction. These energies, depending on the type of problem, may be augmented with reduced volume or bilayer area difference constraints [72]. The mathematical derivation of Canham-Helfrich-type models from molecular descriptions of lipid bilayers by Γ-convergence techniques has been started only recently [10, 64].

Note that for a general membrane $\mathcal{M}$ the Gaussian curvature term $\int_{\mathcal{M}} \kappa_G K$ gives a non-constant contribution to $\mathcal{J}_{CHS}(\mathcal{M})$. However, assuming that $\mathcal{M}$ is closed or that the geodesic curvature along $\partial\mathcal{M}$ is fixed, this term becomes a topological invariant by the Gauss-Bonnet theorem. Hence it can be ignored when computing equilibrium membrane shapes minimizing $\mathcal{J}_{CHS}(\mathcal{M})$.

2.1.1 Monge gauge

We will now outline a geometrically linearised approximation of the Canham-Helfrich energy $\mathcal{J}_{CHS}$ defined in (2.2). The linearisation is used frequently within the physics literature, see for example [72]. For simplicity, let us assume that spontaneous curvature c_0 is zero so that we have

$$\mathcal{J}_{CHS}(\mathcal{M}) = \int_{\mathcal{M}} \tfrac{1}{2}\kappa H^2 + \kappa_G K + \sigma \, d\mathcal{H}^2. \tag{2.3}$$

In the Monge gauge, one assumes that the surface is nearly flat, so that the membrane surface can be parametrized as a graph

$$\mathcal{M} = \{(x_1, x_2, u(x_1, x_2)) \mid (x_1, x_2) \in \Omega\} \tag{2.4}$$

over a two-dimensional reference domain $\Omega \subset \mathbb{R}^2$.

An example of this setting is shown in Figure 2.1. The domain Ω lies in the $x_1 - x_2$ plane with displacements $u(x_1, x_2)$ occurring in the positive x_3-direction. The boundary of Ω is denoted by $\partial\Omega$ and ν denotes the outward pointing unit normal at each point on the boundary.

In the Monge gauge the mean curvature H and the Gauss curvature K of

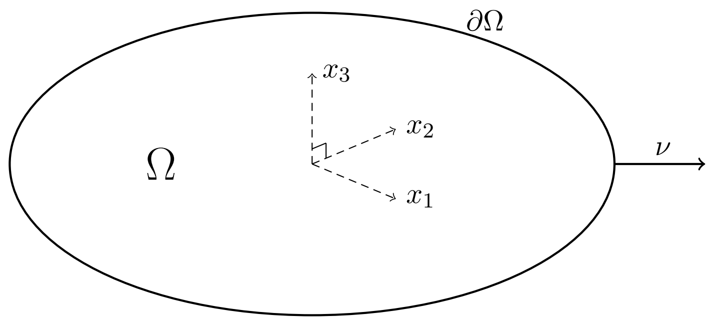


Figure 2.1: The Monge gauge formulation.

the membrane $\mathcal{M}$ are given by

$$H = -\nabla \cdot \frac{\nabla u}{(1+|\nabla u|^2)^{1/2}}, \qquad K = \left(\frac{\partial^2 u}{\partial x_1^2}\frac{\partial^2 u}{\partial x_2^2} - \left(\frac{\partial^2 u}{\partial x_1 \partial x_2}\right)^2 \right) / (1+|\nabla u|^2)^2 \; .$$

A common approach to derive an approximate model is to assume that the displacement of the membrane from the $x-y$ plane produced by the particles is small, i.e. $|\nabla u| \ll 1$. In this case, it is sufficient to consider the geometric linearisation

$$d\mathcal{H}^2 \;\rightsquigarrow\; 1 + \frac{1}{2}|\nabla u|^2 dxdy, \qquad H \;\rightsquigarrow\; -\Delta u, \qquad K \;\rightsquigarrow\; \frac{\partial^2 u}{\partial x_1^2}\frac{\partial^2 u}{\partial x_2^2} - \left(\frac{\partial^2 u}{\partial x_1 \partial x_2}\right)^2, \tag{2.5}$$

which models perturbations from a flat surface. Inserting the geometric linearisation (2.5) into (2.3) yields the quadratic energy

$$\mathcal{J}(u) = \int_\Omega \tfrac{1}{2}\kappa(\Delta u)^2 + \kappa_G \left(\tfrac{\partial^2 u}{\partial x_1^2}\tfrac{\partial^2 u}{\partial x_2^2} - \left(\tfrac{\partial^2 u}{\partial x_1 \partial x_2}\right)^2 \right) + \tfrac{1}{2}\sigma|\nabla u|^2 \, dx. \tag{2.6}$$

Ignoring Gaussian curvature, a quadratic approximation of the energy $\mathcal{J}_{CHS}$ from (2.3) finally takes the form

$$\mathcal{J}(u) = \int_\Omega \tfrac{1}{2}\kappa(\Delta u)^2 + \tfrac{1}{2}\sigma|\nabla u|^2 \, dx. \tag{2.7}$$

Note that the Gaussian curvature may vary across the membrane, we have merely excluded the integral of Gaussian curvature from the quadratic energy on the basis of the Gauss-Bonnet theorem discussed above. Moreover, integrating by parts shows the linearised form of the Gaussian curvature term vanishes under appropriate boundary conditions, these are discussed in the next section. Observe that minimization of $\mathcal{J}$ leads to fourth order plate-like equations. This technique of linearisation is informally justified and generalised to graphs over curved surfaces in Chapter 4.

2.1.2 Boundary conditions and coercivity

We consider the Canham-Helfrich free energy $\mathcal{J}(u)$ in the Monge gauge (2.7) with membrane displacement u defined on a reference domain $\Omega \subset \mathbb{R}^2$. In this chapter we assume that $\Omega \subset \mathbb{R}^2$ is a bounded domain with a piecewise smooth Lipschitz boundary $\partial\Omega$, e.g., a square. Deformations u of the membrane are taken from a closed subspace $V \subset H^2(\Omega)$ satisfying suitable boundary conditions. We consider the following three cases

$$V = H_0^2(\Omega), \qquad V = H^2(\Omega) \cap H_0^1(\Omega), \qquad V = H_{p,0}^2(\Omega), \tag{2.8}$$

often referred to as Dirichlet, Navier, and periodic boundary conditions with zero mean, respectively. Note that

$$H_{p,0}^2(\Omega) = \overline{\{v|_\Omega \mid v \in C^\infty(\mathbb{R}^2) \text{ is } \Omega\text{-periodic and } \int_\Omega v \, ds = 0\}}.$$

is only defined for a rectangular domain Ω. The space V is equipped with the canonical norm $\|\cdot\|_2 = \|\cdot\|_{H^2(\Omega)}$ in $H^2(\Omega)$. Throughout the following, we assume that $\kappa > 0$ and $\sigma \geq 0$ for all three choices of V.

Lemma 2.1.1. *The bilinear form*

$$a(v, w) = \int_\Omega \kappa \Delta v \Delta w \, dx + \sigma \nabla v \cdot \nabla w \, dx, \qquad v, w \in V,$$

associated with the energy functional $\mathcal{J}$ is continuous and coercive on V.

Proof. While continuity of $a(\cdot, \cdot)$ is obvious, we refer to Appendix B for a proof of coercivity. □

In the biophysics literature problems in the Monge gauge are frequently studied over the whole space $\Omega = \mathbb{R}^2$ with the boundary conditions that the membrane is asymptotically flat, that is $u(x), |\nabla u(x)| \to 0$ as $|x| \to \infty$. The Dirichlet and Navier boundary conditions are interpretations of this for finite size domains. For the Dirichlet boundary conditions $u = |\nabla u| = 0$ holds along $\partial\Omega$. The Navier boundary conditions give rise to a variational problem whose solution satisfies $u = \Delta u = 0$ on $\partial\Omega$. The second condition can be seen as an approximation of the mean curvature H vanishing on the boundary, which is another way in which flatness of the membrane may be characterised.

2.1.3 Interactions with the cytoskeleton

We will consider interactions of the membrane with thin actin filaments that are anchored to the cytoskeleton and may prescribe displacements of the membrane or with particles that apply forces that may be due to either entropic or direct chemical interactions (see, e.g., [33, 37]). In the mathematical models to be considered in this chapter these effects are represented by point value constraints or point forces.

2.2 Point value constraints

2.2.1 Point value constraints at fixed locations

Prescribed point values at N given locations $X = (X_i) \in \overline{\Omega}^N$ are represented by the constraints

$$F_X u = \alpha \tag{2.9}$$

with given $\alpha \in \mathbb{R}^N$ and $F_X = (F_{X,i}) : V \to \mathbb{R}^N$ defined by

$$F_{X,i} v = \delta_{X_i} v \in \mathbb{R}, \tag{2.10}$$

as illustrated in Figure 2.2. Note that $\delta_{X_i} \in V^*$ and thus $F_X \in (V^*)^N$ due to

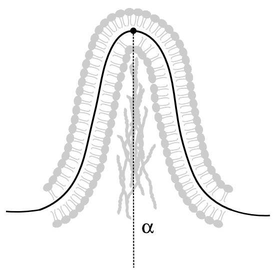


Figure 2.2: Displacements caused by filaments anchored in the cytoskeleton.

the continuous embedding $V \subset H^2(\Omega) \subset C(\overline{\Omega})$. We first consider prescribed point values at fixed locations.

Problem 2.2.1 (Point value constraints)**.**
Find $u \in V$ minimising the energy $\mathcal{J}$ on V subject to the constraints (2.9)*.*

In order to avoid possible conflicts of point constraints (2.9) with boundary conditions (2.8), we exclude $X_i \in \partial\Omega$.

Proposition 2.2.1. *For distinct locations $X_1, \ldots, X_N \in \Omega$ there exists a unique solution $u \in V$ to Problem 2.2.1.*

Proof. As the locations $X_1, \ldots, X_N$ are distinct and contained in Ω the functionals δ_{X_i} are linearly independent for all three choices (2.8) of V. Hence, the assertion follows from Proposition A.1.1. $\square$

Remark 2.2.1. *In applying Proposition A.1.1, we can also derive a representation of the solution in terms of Green's functions $\phi_i \in V$, defined by*

$$a(\phi_i, v) = \delta_{X_i}(v) \quad \forall v \in V, \qquad i = 1, \ldots, N.$$

2.2.2 Point value constraints with varying locations

Existence of global minimizers

We now seek a global minimizer over prescribed point values in the sense that we allow for varying locations $X = (X_i) \in \overline{\Omega}^N$. This can be viewed as finding the optimal locations for filaments which prescribe a particular set of displacements.

Problem 2.2.2 (Point value constraints with varying locations)**.**
Find $(u, X) \in V \times \overline{\Omega}^N$ such that u is minimising the energy $\mathcal{J}$ on V subject to the constraint

$$F_X u = \alpha$$

with given $\alpha \in \mathbb{R}^N$.

Lemma 2.2.1. *The mapping $\overline{\Omega} \ni X_i \to \delta_{X_i} \in (V^*)$ and thus the mapping $\overline{\Omega}^N \ni X \to F_X \in (V^*)^N$ is continuous.*

Proof. Since the Sobolev embedding theorem provides continuity of the injection $V \subset H^2(\Omega) \to C^{0,\lambda}(\overline{\Omega})$ for any Hölder-exponent $0 < \lambda < 1$ (see, e.g., [1, Theorem 4.12]), the estimate

$$|(\delta_{X_i} - \delta_{Y_i})v| = |v(X_i) - v(Y_i)| \leq \|v\|_{C^{0,\lambda}} |X_i - Y_i|^\lambda \leq C\|v\| |X_i - Y_i|^\lambda$$

holds for each $i = 1, \ldots, N$. Thus $\|\delta_{X_i} - \delta_{Y_i}\|_{(V^*)^N} \to 0$ as $X \to Y$. $\square$

Proposition 2.2.2. *There exists a solution $(u, X) \in V \times \overline{\Omega}^N$ to Problem 2.2.2.*

Proof. It is well-known that $\overline{\Omega}^N \in \mathbb{R}^N$ is compact. Furthermore, the mapping $\overline{\Omega}^N \ni Y \to F_Y \in (V^*)^N$ is continuous by Lemma 2.2.1 and $V_{\alpha,Y} = \{v \in V \mid F_Y v = \alpha\}$ is non-empty for some $Y = (Y_i) \in \overline{\Omega}^N$, e.g. for pairwise distinct locations $Y_i \in \Omega$. Now the assertion follows from Proposition A.1.2. □

Remark 2.2.2. *Existence of a solution of a penalized version of Problem 2.2.2 follows from Proposition A.2.1 in complete analogy to penalized curvature constraints as considered in Problem 3.2.3.*

Characterisation of global minimizers

Having shown the existence of global minimizers we will now produce equivalent characterisations of solutions. First, we note considerable simplifications of Problem 2.2.2 depending upon the signs of the prescribed point values.

Proposition 2.2.3. *Assume that the prescribed point values have the same sign and let $0 \le |\alpha_1| \le \cdots \le |\alpha_N|$. Then $(u, X) \in V \times \overline{\Omega}^N$ is a solution of Problem 2.2.2, if and only if $(u, X_N) \in V \times \overline{\Omega}$ solves Problem 2.2.2 with $N = 1$ and $\alpha = \alpha_N$.*

Proof. The solution of Problem 2.2.2 is equivalent to solve

$$u = \operatorname*{arg\,min}_{v \in V_{\alpha,N}} \mathcal{J}(v), \qquad V_{\beta,k} = \{v \in V \mid \exists Y \in \overline{\Omega}^k : \ \ \delta_{Y_i} v = \beta_i \text{ for } i = 1, \ldots, k\},$$

and to take $X \in \overline{\Omega}^N$ such that $F_X u = \alpha$. Hence, it is sufficient to show that $V_{\alpha,N} = V_{\alpha_N,1}$. The inclusion $V_{\alpha,N} \subset V_{\alpha_N,1}$ is obvious by definition. It remains to show $V_{\alpha_N,1} \subset V_{\alpha,N}$.

To this end let $v \in V_{\alpha_N,1}$ and $X_N \in \overline{\Omega}$ such that $v(X_N) = \alpha_N$. Then, by continuity of v on $\overline{\Omega}$, for all three choices (2.8) of V there is $X_0 \in \overline{\Omega}$ with $v(X_0) = 0$. Now, by continuity of v and the connectedness of $\overline{\Omega}$, the intermediate value theorem implies that v attains each value $\alpha_i \in [0, \alpha_N]$ at some point $X_i \in \overline{\Omega}$ and hence $v \in V_{\alpha,N}$. □

We now move on to the case where the prescribed point values α_i do not have the same sign. Similarly to the previous case, the behaviour is governed by the extreme values of α, in this case the greatest and least.

Proposition 2.2.4. *Let $\alpha_1 \le ... \le \alpha_N$. Then $(u, X) \in V \times \overline{\Omega}^N$ is a solution of Problem 2.2.2, if and only if $(u, (X_1, X_N)) \in V \times \overline{\Omega}^2$ solves Problem 2.2.2 with $N = 2$ and $\alpha = (\alpha_1, \alpha_N)$.*

Proof. Utilizing the notation as introduced in the proof of Proposition 2.2.3, it is sufficient to show $V_{\alpha,N} = V_{(\alpha_1,\alpha_N),2}$. While $V_{\alpha,N} \subset V_{(\alpha_1,\alpha_N),2}$ is obvious by definition, the converse inclusion again follows by connectedness of $\overline{\Omega}$, continuity of $v \in V$, and the intermediate value theorem. □

We have thus reduced N to one or two constraints, based upon the signs of the prescribed point values. We first concentrate on the case of point values with the same sign and reformulate Problem 2.2.2 in terms of the Green's function $\phi_x \in V$, defined by

$$a(\phi_x, v) = \delta_x v \quad \forall v \in V, \qquad x \in \overline{\Omega}. \tag{2.11}$$

By definition, $a(\phi_x, \phi_x) = \phi_x(x)$ holds for all $x \in \overline{\Omega}$. In order to exclude the degenerate case $\phi_x = 0$ we will constrain x to the set

$$\Omega_V = \{x \in \overline{\Omega} \mid \phi_x(x) \neq 0\}.$$

Notice that Ω_V depends on the choices (2.8) of the boundary conditions incorporated in V: For $V = H_0^2(\Omega)$ and $V = H^2(\Omega) \cap H_0^1(\Omega)$ we have $\Omega_V = \Omega$ whereas $V = H_{p,0}^2(\Omega)$ allows for $\Omega_V = \overline{\Omega}$.

Proposition 2.2.5. *Assume that the prescribed point values have the same sign and let* $0 \leq |\alpha_1| \leq \cdots \leq |\alpha_N|$. *Then the solution of Problem 2.2.2 is given by*

$$X_N = \operatorname*{arg\,min}_{x \in \Omega_V} \frac{\alpha_N^2}{\phi_x(x)}, \qquad u = \frac{\alpha_N}{\phi_{X_N}(X_N)} \phi_{X_N} \tag{2.12}$$

and $X_1, \ldots, X_{N-1}$ *such that* $u(X_i) = \alpha_i$, $i = 1, \ldots, N-1$.

Proof. First we note that (2.12) is well-defined because we have $\phi_x(x) \neq 0$ for $x \in \Omega_V$. Proposition 2.2.3 implies that the solution u of Problem 2.2.2 is the minimizer of $\mathcal{J}$ subject to the constraint that $\delta_{X_N} u = \alpha_N$ holds with some $X_N \in \overline{\Omega}$. For $\alpha_N = 0$ we only have the trivial minimizer $u = 0$ which is in accordance with (2.12).

Now let $\alpha_N \neq 0$. For $x \in \overline{\Omega} \setminus \Omega_V$ we have $\delta_x v = 0 \neq \alpha_N$ for all $v \in V$. Hence we must have $X_N \in \Omega_V$ for all solutions (u, X_N) and the representation (2.12) follows from Lemma A.1.3. □

Note that in the generic case $\alpha_N \neq 0$, the optimal location X_N is independent of α_N and u depends linearly on α_N.

If the prescribed point values do not have the same sign, then Problem 2.2.2 can be reformulated in terms of two Green's functions ϕ_{Y_1}, $\phi_{Y_2} \in V$ defined by

$$a(\phi_{Y_1}, v) = \delta_{Y_1}(v), \quad a(\phi_{Y_2}, v) = \delta_{Y_2}(v) \qquad \forall v \in V, \qquad\qquad (Y_1, Y_2) \in \overline{\Omega}^2,$$

and the associated Gramian matrix $A_Y = (a(\phi_{Y_j}, \phi_{Y_i})) = (\phi_{Y_i}(Y_j))$.

Proposition 2.2.6. *Let $\alpha_1 \leq \cdots \leq \alpha_N$ and assume that $\alpha_1 < 0 < \alpha_N$. Then the solution of Problem 2.2.2 is given by*

$$(X_1, X_N) = \operatorname*{arg\,min}_{Y \in \Omega_V^2, Y_1 \neq Y_2} (\alpha_1, \alpha_N) A_Y^{-1} (\alpha_1, \alpha_N)^\top, \tag{2.13}$$

$$u = U_1 \phi_{X_1} + U_2 \phi_{X_N} \qquad U = A_{(X_1, X_N)}^{-1} (\alpha_1, \alpha_N)^\top \in \mathbb{R}^2, \tag{2.14}$$

and $X_2, \ldots, X_{N-1}$ such that $u(X_i) = \alpha_i$, $i = 2, \ldots, N-1$.

Proof. First we note that A_Y is regular and (2.13), (2.14) are well-defined because we have $\phi_{Y_1} \neq 0 \neq \phi_{Y_2}$ and $\phi_{Y_1} \neq \phi_{Y_2}$ for $Y \in \mathcal{M}' = \{Y \in \Omega_V^2 \mid Y_1 \neq Y_2\}$.

Proposition 2.2.4 implies that the solution $u \in V$ of Problem 2.2.2 is the minimizer of $\mathcal{J}$ subject to the constraints that $\delta_{X_1} u = \alpha_1$, $\delta_{X_N} u = \alpha_N$ hold with some $(X_1, X_N) \in \overline{\Omega}^2$. For $Y \in \overline{\Omega}^2 \setminus \mathcal{M}'$ we either have $Y_i \in \overline{\Omega} \setminus \Omega_V$ for some i and hence $\alpha_1 < \delta_{Y_i} v = 0 < \alpha_N$ for all $v \in V$ or we have $Y_1 = Y_2$ and thus $\delta_{Y_1} = \delta_{Y_2}$ such that there is again no $v \in V$ that satisfies the constraints $\delta_{Y_1} v = \alpha_1 < \alpha_N = \delta_{Y_2} v$. Hence, $(X_1, X_N) \in \mathcal{M}'$ must hold for all solutions $(u, (X_1, X_N))$ of Problem 2.2.2. Now the representation (2.13), (2.14) follows from Lemma A.1.3. □

Note that the locations X_i do depend on the α_i even though the minimising function u depends only upon α_N in the same sign case and on α_1, α_N in the opposite sign case. In addition, If the assumption $\alpha_1 < 0 < \alpha_N$ is not fulfilled then all α_i have the same sign. In this case we can use the representation given by Proposition 2.2.5.

2.3 Point forces

2.3.1 Point forces at fixed locations

We now consider forces exerted on the membrane that are localized to certain points $X_i \in \overline{\Omega}$, $i = 1, \ldots, N$. These forces are perpendicular to Ω with positive or negative direction and give rise to the additional term

$$\ell_X(u) = \sum_{i=1}^{N} \beta_i \delta_{X_i} u \tag{2.15}$$

in the energy functional to be minimized. Here, $\beta_i \in \mathbb{R} \setminus \{0\}$ are given constants representing the magnitude of point forces at the locations X_i. We set

$$\mathcal{E}(u, X) = \mathcal{J}(u) - \ell_X(u), \qquad u \in V, \quad X \in \overline{\Omega}^N$$

with the closed subspace $V \subset H^2(\Omega)$ defined in (2.8) and consider the following minimization problem.

Problem 2.3.1 (Point forces at fixed locations)**.**
For given $X = (X_i) \in \overline{\Omega}^N$ *find* $u \in V$ *minimising the energy* $\mathcal{E}(u, X)$ *on* V*.*

Existence and uniqueness of a solution $u \in V$ of Problem 2.3.1 follows from the Lax-Milgram lemma. It is characterised by the variational equality

$$a(u, v) = \ell_X(v) \qquad \forall v \in V. \tag{2.16}$$

The solution can be represented by Green's functions ϕ_x as defined in (2.11).

Lemma 2.3.1. *For given* $X \in \overline{\Omega}^N$ *the solution* $u \in V$ *of Problem 2.3.1 is given by*

$$u = \sum_{i=1}^{N} \beta_i \phi_{X_i}.$$

Proof. The assertion follows directly from the linear representation (2.15) of ℓ_X by the functionals δ_{X_i}. □

2.3.2 Point forces at varying locations

Existence of global minimizers

We now seek a global minimizer over prescribed point forces, in the sense that we allow the point forces to be applied at varying locations $X = (X_i) \in \overline{\Omega}^N$.

Problem 2.3.2 (Point forces at varying locations)**.**
Find $(u, X) \in V \times \overline{\Omega}^N$ *minimising the energy* $\mathcal{E}$ *on* $V \times \overline{\Omega}^N$*.*

Proposition 2.3.1. *There exists a solution* $(u, X) \in V \times \overline{\Omega}^N$ *to Problem 2.3.2.*

Proof. In light of the continuity of $\overline{\Omega} \ni X_i \to \delta_{X_i} \in V^*$ as stated in Lemma 2.2.1, the assertion follows from Proposition A.1.3. □

In general, there is no uniqueness of solutions of Problem 2.3.2. For example, let $N = 2$, $\beta_2 = -\beta_1$, and assume that $(u, (X_1, X_2))$ is a solution of Problem 2.3.2. Then $(-u, (X_2, X_1))$ is another solution.

Using the representation for fixed X given in Lemma 2.3.1, we will also construct a representation of solutions to Problem 2.3.2. To this end, we from now on denote by $u_Y \in V$ the unique minimizer of $\mathcal{E}(\,\cdot\,, Y)$ for given $Y \in \overline{\Omega}^N$. As a first step, we compute the energy of such minimizers.

Lemma 2.3.2. *Let $Y \in \overline{\Omega}^N$ be given and $A_Y = (a(\phi_{Y_i}, \phi_{Y_j})) \in \mathbb{R}^{N\times N}$. Then*

$$\min_{v\in V} \mathcal{E}(v, Y) = \mathcal{E}(u_Y, Y) = -\tfrac{1}{2}a(u_Y, u_Y) = -\tfrac{1}{2}\ell_Y(u_Y) = -\tfrac{1}{2}\beta^\top A_Y \beta. \tag{2.17}$$

Proof. After inserting $v = u_Y$ into the variational equality (2.16) for u_Y, we use the definition of ℓ_Y, and the representation of u_Y as given in Lemma 2.3.1 to obtain

$$\mathcal{E}(u_Y, Y) = -\tfrac{1}{2}a(u_Y, u_Y) = -\tfrac{1}{2}\ell_Y(u_Y) = -\tfrac{1}{2}\sum_{i=1}^{N} \beta_i u_Y(Y_i) = -\tfrac{1}{2}\sum_{i,j=1}^{N} \beta_i\beta_j\phi_{Y_j}(Y_i).$$

Now definition (2.11) of the Green's functions ϕ_{Y_i} yields $(A_Y)_{i,j} = a(\phi_{Y_i}, \phi_{Y_j}) = \phi_{Y_j}(Y_i)$. This completes the proof. $\square$

As a direct consequence we get the following characterisation of Problem 2.3.2.

Proposition 2.3.2. *Let $A_Y \in \mathbb{R}^{N\times N}$ as in Lemma 2.3.2. Then $(u, X) \in V \times \overline{\Omega}^N$ minimizes $\mathcal{E}$, if and only if $u = u_X$ with X minimizing the function*

$$\overline{\Omega}^N \ni Y \mapsto -\tfrac{1}{2}\beta^\top A_Y \beta \in \mathbb{R}.$$

Clustering

Having established the existence of global minimizers we will now explore the properties of minimizers for particular combinations of the parameters β_i, $i = 1, \dots, N$. Of particular interest will be exhibiting cases where optimal locations of point forces lie inside Ω. Of course, this is of no interest under periodic boundary conditions as it is the zero boundary condition in the other two sets of boundary conditions which causes point forces to have no effect along the boundary. As such, we will assume $V = H_0^2(\Omega)$ or $V = H^2(\Omega) \cap H_0^1(\Omega)$ for the rest of this section, but will remark where this assumption plays a role. We will also show clustering behaviour for larger numbers of point forces and that opposite point forces do not annihilate each other.

We first show that point forces do not cluster on the boundary $\partial\Omega$ of Ω.

Lemma 2.3.3. *Assume that $(u, X) \in V \times \overline{\Omega}^N$ is a solution of Problem 2.3.2. Then $\mathcal{E}(u, X) < 0$ and $X \notin (\partial\Omega)^N$.*

Proof. Assume that $(u, X) \in V \times (\partial\Omega)^N$ solves Problem 2.3.2. Then $\ell_X(v) = 0$ holds for all $v \in V$ and therefore $u = u_X = 0$. Hence, we have

$$\mathcal{E}(u, X) = -\tfrac{1}{2}a(u, u) = 0 > -\tfrac{1}{2}a(u_Y, u_Y) = \mathcal{E}(u_Y, Y)$$

for $Y = (Y_i)$ with $Y_1 \in \Omega$ and $Y_i = X_i$, $i = 2, \ldots, N$. This contradicts optimality of (u, X). $\square$

The following lemma quantifies the change of energy that is caused by moving a single point force. This is the key ingredient to prove clustering of point forces later on.

Lemma 2.3.4. *Let $X, Y \in \overline{\Omega}^N$ and assume $Y_i = X_i$ for $i \neq k$ with some fixed k. Then*

$$\mathcal{E}(u_Y, Y) = \mathcal{E}(u_X, X) - \beta_k(\delta_{Y_k} - \delta_{X_k})(u_X) - \tfrac{1}{2}\beta_k^2 a(\phi_{Y_k} - \phi_{X_k}, \phi_{Y_k} - \phi_{X_k}).$$

Proof. The representation of energy in Lemma 2.3.2 and the binomial formula provide the estimate

$$\mathcal{E}(u_Y, Y) = \mathcal{E}(u_X, X) - (\ell_Y - \ell_X)(u_X) - \tfrac{1}{2}a(u_Y - u_X, u_Y - u_X) \tag{2.18}$$

for any $X, Y \in \overline{\Omega}^N$. Now let $X_i = Y_i$ for $i \neq k$. Then we have $\ell_Y = \ell_X + \beta_k(\delta_{Y_k} - \delta_{X_k})$ and $u_Y = u_X + \beta_k(\phi_{Y_k} - \phi_{X_k})$. Inserting these identities into (2.18) we obtain the assertion. $\square$

In the forthcoming clustering analysis we will make use of the equivalence relation

$$x \mathrel{\widehat{=}} y \quad \Leftrightarrow \quad \delta_x v = \delta_y v \ \ \forall v \in V. \tag{2.19}$$

Recall that we have $\delta_x = 0$ on V for all $x \in \partial\Omega$. Hence, $x \mathrel{\widehat{=}} y$ holds, if and only if $x = y$ or $x, y \in \partial\Omega$. By definition, the locations of a solution can be replaced by equivalent locations.

Lemma 2.3.5. *Assume that $(u, X) \in V \times \overline{\Omega}^N$ is a solution of Problem 2.3.2 and that $Y_i \mathrel{\widehat{=}} X_i$ holds for all $i = 1, \ldots, N$. Then $(u, Y) \in V \times \overline{\Omega}^N$ is also a solution of Problem 2.3.2.*

Now we are ready to prove clustering of point forces.

Proposition 2.3.3. *Assume that* $(u, X) \in V \times \overline{\Omega}^N$ *is a solution to Problem 2.3.2. Then there exist* $(X^+, X^-) \in \overline{\Omega}^2$ *such that* $(X^+, X^-) \notin (\partial\Omega)^2$ *and*

$$\beta_i > 0 \ \Rightarrow \ X_i \mathrel{\widehat{=}} X^+, \qquad \beta_i < 0 \ \Rightarrow \ X_i \mathrel{\widehat{=}} X^- \tag{2.20}$$

holds for all $i = 1, \ldots, N$.

Proof. Let $(u_X, X) \in V \times \overline{\Omega}$ be a solution of Problem 2.3.2. Then we have

$$\beta_i \delta_{X_i}(u_X) \geq 0 \qquad \forall i = 1, \ldots, N. \tag{2.21}$$

Indeed, if there is a k such that $\beta_k \delta_{X_k}(u_X) < 0$ then we can chose $Y_i = X_i$, $i \neq k$ and $Y_k \in \partial\Omega$ to obtain the contradiction $\mathcal{E}(u_Y, Y) < \mathcal{E}(u_X, X)$ from Lemma 2.3.4.

Recall that Lemma 2.3.3 implies $X \notin (\partial\Omega)^N$. Hence, at least one point force must be located in Ω. Let $X_j \in \Omega$ be arbitrarily chosen. Then it is sufficient to show that $X_i = X_j$ must hold for all $i \in \mathcal{I}_j = \{l = 1, \ldots, N \mid \operatorname{sgn}(\beta_l) = \operatorname{sgn}(\beta_j)\}$.

Without loss of generality assume that $\beta_j > 0$ and that j is selected such that $\delta_{X_j}(u_X) \geq \delta_{X_i}(u_X)$ holds for all other $X_i \in \Omega$ with $i \in \mathcal{I}_j$.

In contradiction to the assertion, we now assume that $X_k \neq X_j$ holds for some $k \in \mathcal{I}_j$. Application of Lemma 2.3.4 with $Y_i = X_i$, $i \neq k$ and $Y_k = X_j$, together with $\delta_{X_j}(u_X) \geq \delta_{X_k}(u_X)$ provides

$$\begin{aligned} \mathcal{E}(u_Y, Y) &= \mathcal{E}(u_X, X) - \beta_k(\delta_{X_j} - \delta_{X_k})(u_X) - \tfrac{1}{2}\beta_k^2 a(\phi_{X_j} - \phi_{X_k}, \phi_{X_j} - \phi_{X_k}) \\ &\leq \mathcal{E}(u_X, X) - \tfrac{1}{2}\beta_k^2 a(\phi_{X_j} - \phi_{X_k}, \phi_{X_j} - \phi_{X_k}). \end{aligned}$$

Now we have either $X_k \in \partial\Omega$, and therefore $\phi_{X_k} = 0$, or $X_k \in \Omega$, and therefore that ϕ_{X_k} and ϕ_{X_j} are linearly independent. In both cases $a(\phi_{X_j} - \phi_{X_k}, \phi_{X_j} - \phi_{X_k}) > 0$ providing $\mathcal{E}(u_Y, Y) < \mathcal{E}(u_X, X)$. This contradicts optimality of (u_X, X). $\square$

Remark 2.3.1. *As a consequence of Proposition 2.3.3, the point forces with positive (negative) sign either cluster in one point* $X^+ \in \Omega$ $(X^- \in \Omega)$ *or are all located on the boundary* $\partial\Omega$. *By Lemma 2.3.3, not all* N *point forces can be located on the boundary. Hence point forces of a solution* (u, X) *of Problem 2.3.2 cluster in exactly one of the following three ways.*

(i) $X_i = X^+ \in \Omega$ *for all* i *with* $\beta_i > 0$ *and* $X_i = X^- \in \Omega$ *for all* i *with* $\beta_i < 0$,

(ii) $X_i = X^+ \in \Omega$ *for all* i *with* $\beta_i > 0$ *and* $X_i \in \partial\Omega$ *for all* i *with* $\beta_i < 0$,

(iii) $X_i = X^- \in \Omega$ *for all* i *with* $\beta_i < 0$ *and* $X_i \in \partial\Omega$ *for all* i *with* $\beta_i > 0$.

We may regard the occurrence of one of these three cases as a property of $a(\cdot,\cdot)$, the parameters β_i, and Ω.

As another consequence of Proposition 2.3.3 we can characterise the solutions to Problem 2.3.2 with N forces in terms of an equivalent problem with at most two forces.

Corollary 2.3.1. *Let*

$$\beta^+ = \sum_{\beta_i>0} \beta_i \geq 0, \qquad \beta^- = \sum_{\beta_i<0} \beta_i \leq 0. \tag{2.22}$$

Then $(u, X) \in V \times \overline{\Omega}^N$ is a solution of Problem 2.3.2 with $(X^+, X^-) \in \overline{\Omega}^2$ satisfying (2.20), *if and only if $(u, (X^+, X^-)) \in V \times \overline{\Omega}^2$ is a solution of Problem 2.3.2 with point forces*

$$\ell_{X_0} = \beta^+\delta_{X^+} + \beta^-\delta_{X^-}, \qquad X_0 = (X^+, X^-).$$

Proof. Proposition 2.3.3 implies that the locations X of all solutions to Problem 2.3.2 are contained in the subset

$$M = \left\{ X \in \overline{\Omega}^N \mid \exists (X^+, X^-) \in \overline{\Omega}^2 \text{ with (2.20) } \right\} \subset \overline{\Omega}^N.$$

Hence minimizing $\mathcal{E}(u, X)$ over $V \times \overline{\Omega}^N$ is equivalent to minimization over $V \times M$.

By definition of M, we can identify M with $\overline{\Omega}^2$ by the condition (2.20) up to componentwise equivalence in the sense of (2.19). Now, let $X \in M$ be identified with $X_0 = (X^+, X^-) \in \overline{\Omega}^2$ in this way. As a consequence of (2.20), we then have $\ell_X = \ell_{X_0}$ and thus $u_X = u_{X_0}$. In light of Lemma 2.3.2, this leads to

$$\begin{aligned} \mathcal{E}(u_X, X) &= -\tfrac{1}{2}a(u_X, u_X) = -\tfrac{1}{2}a(u_{X_0}, u_{X_0}) \\ &= \mathcal{J}(u_{X_0}) - \ell_{X_0}(u_{X_0}) =: \mathcal{E}_0(u_{X_0}, X_0) \end{aligned}$$

Therefore, minimization of $\mathcal{E}(u, X)$ over $V \times M$ is equivalent to minimization of the energy $\mathcal{E}_0(u_{X_0}, X_0)$ over $V \times \overline{\Omega}^2$. This concludes the proof. $\square$

By Proposition 2.3.3 at least one of the clustering points X^+, $X^- \in \overline{\Omega}$ must be contained in Ω. Utilizing the values of β^+ and β^- defined in (2.22), we can often exclude one of the three cases in Remark 2.3.1.

Proposition 2.3.4. *Let (u, X) be a solution of Problem 2.3.2. If $|\beta^+| > |\beta^-|$, then $X^+ \in \Omega$ and if $|\beta^+| < |\beta^-|$, then $X^- \in \Omega$.*

Proof. Let (u_X, X) be a solution of Problem 2.3.2 and $|\beta^+| > |\beta^-|$. In contradiction to the assertion, we assume that $X^+ \in \partial\Omega$. Then, Lemma 2.3.3 yields $X^- \in \Omega$ and thus $\delta_{X^-} \neq 0$. In addition, Corollary 2.3.1 implies that $(u_X, (X^+, X^-))$ is a minimizer of the energy $\mathcal{E}_0 = \mathcal{J} - \ell_{X_0}$ on $V \times \overline{\Omega}^2$. From $X^+ \in \partial\Omega$, we get $u_X = \beta^- \phi_{X_-}$. This leads to

$$\begin{aligned}\mathcal{E}_0(u_X, (X^+, X^-)) &= -\tfrac{1}{2}|\beta^-|^2 a(\phi_{X^-}, \phi_{X^-}) \\ &> -\tfrac{1}{2}|\beta^+|^2 a(\phi_{X^-}, \phi_{X^-}) = \mathcal{E}_0(u_{(X^-,X^+)}, (X^-, X^+))\end{aligned}$$

in contradiction to the optimality of $(u_X, (X^+, X^-))$. In the remaining case $|\beta^+| < |\beta^-|$ the assertion follows by symmetry. $\square$

We now assume that all forces point in the same direction. In this case, the solutions of Problem 2.3.2 can be obtained by solving Problem 2.3.2 with a single force.

Corollary 2.3.2. *Assume that all of the coefficients β_i have the same sign. Then $(u, X) \in V \times \overline{\Omega}^N$ is a solution to Problem 2.3.2, if and only if $X_1 = \cdots = X_N \in \Omega$ and (u, X_1) is a solution of Problem 2.3.2 with one point force*

$$\ell_{X_1} = \Big(\sum_{i=1}^{N} \beta_i\Big) \delta_{X_1}.$$

Proof. By Lemma 2.3.3 there must be at least one $X_k \in \Omega$. Then, Proposition 2.3.3 provides $X_1 = \cdots = X_k = \cdots = X_N$ and the assertion follows from Corollary 2.3.1. $\square$

We have thus characterised the behaviour of systems with forces that are all pointing in one direction: The global minimizer is simply when all of the particles lie at the same point and that point is a global minimizer for only one point force. There is still no uniqueness however, as global minimizers for the one point force problem are not unique in general. The uniqueness for the one point force problem may be regarded as a property of the domain Ω. For example, we will explicitly calculate the solution to the one point force problem for $\Omega = B(0, 1)$ in (2.25). From this expression it is clear that we have uniqueness when Ω is circular. By numerical experiments (not fully detailed here) we have considered a 'bowtie' shaped domain as shown in Figure 2.3. In this case it appears the one point force problem does not admit a unique global minimizer, as point forces located as indicated in the figure produce equal, minimal energies.

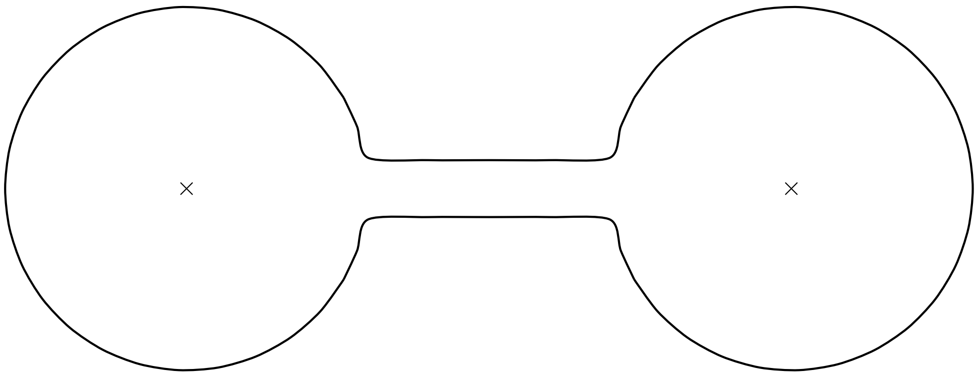


Figure 2.3: A bowtie shaped domain

Remark 2.3.2. *All results given above can be extended to the case* $V = H^2_{p,0}(\Omega)$ *by replacing all occurrences of* Ω *by* $\overline{\Omega}$ *and dropping all cases where* $\partial\Omega$ *shows up.*

2.3.3 Discussion

The models formulated in Problem 2.2.1 and Problem 2.2.2 describe the optimal shape of a membrane under point constraints and the optimal location of such constraints. This approach could be used to describe the action of actin filaments bound to the membrane. Such kind of problems also occur in the study of thin plates. For example, Problem 2.2.1 is the central object in the study of thin plate splines and Problem 2.2.2 is analysed in [12] which studies support points of a plate, producing this problem with homogeneous data $\alpha = 0$.

The model set out in Problem 2.3.1 and further extended and analysed in Section 2.3.2 is motivated by the general approach in [33] where protein membrane interaction is described by an additional term in the membrane energy functional representing the work done by the pressure exerted by proteins. In [33] the particles are assumed to have a positive diameter and are bound to membrane. We have adapted this model to particles anchored to the cytoskeleton applying point forces. Note that the results on clustering of point forces, derived above, do not agree with the interaction of finite sized particles, as investigated in [33]. The key difference between the two models is that the point forces in Problem 2.3.2 do apply a net force to the membrane which is not the case for the interactions studied in [33]. The action of protrusive forces on a membrane is discussed in [37, 77]. The variational framework we have introduced may be also applied in this case and used to analyse the membrane mediated interactions between particles.

2.4 Numerical experiments

2.4.1 Finite element method

We consider Problem 2.3.1 with point forces at fixed locations $X = (X_i) \in \overline{\Omega}$ with the solution space $V = H^2(\Omega) \cap H_0^1(\Omega)$. The numerical approach is based on a splitting of the fourth order problem (2.16) into two second order problems for the unknown functions u and $w = \kappa\Delta u - \sigma u$. This method requires the regularity result in Lemma C.1.1 and thus we will assume Ω is convex for the remainder of this chapter. To make the splitting method rigorous we require the following reformulation of (2.16).

Problem 2.4.1. *Let $p \in (2, \infty)$ and $q \in (1, 2)$ be chosen such that $1/p + 1/q = 1$. Find $(u, w) \in H_0^1(\Omega) \times W_0^{1,q}(\Omega)$ such that*

$$\int_\Omega \nabla w \cdot \nabla v = -\sum_{i=1}^N \beta_i \delta_{X_i} v \quad \forall v \in W_0^{1,p}(\Omega), \tag{2.23}$$

$$\int_\Omega \kappa \nabla u \cdot \nabla v + \sigma u v = -\int_\Omega wv \qquad \forall v \in H_0^1(\Omega). \tag{2.24}$$

Lemma 2.4.1. *There exists a unique solution to Problem 2.4.1.*

Proof. The well posedness of (2.23) is given in [14, Theorem 2]. As the equations are decoupled well posedness of (2.24) then follows by the Lax-Milgram theorem. □

The following lemma proves the equivalence of this problem and Problem 2.3.1.

Lemma 2.4.2. *The pair $(u, w) \in H_0^1(\Omega) \times W_0^{1,q}(\Omega)$ solves Problem 2.4.1 if and only if u solves Problem 2.3.1 with $V = H^2(\Omega) \cap H_0^1(\Omega)$ and $w = \kappa\Delta u - \sigma u$.*

Proof. Suppose $(u, w) \in H_0^1(\Omega) \times W_0^{1,q}(\Omega)$ solves Problem 2.4.1. Applying elliptic regularity gives $u \in V$ and $w = \kappa\Delta u - \sigma u$. Thus for any $v \in V$, $v \in W_0^{1,p}(\Omega)$ and hence

$$\int_\Omega \kappa \Delta u \Delta v + \sigma \nabla u \cdot \nabla v = \int_\Omega w \Delta v = -\int_\Omega \nabla w \cdot \nabla v = \sum_{i=1}^N \beta_i \delta_{X_i} v.$$

Thus u solves Problem 2.3.1.

Now suppose u solves Problem 2.3.1 with $V = H^2(\Omega) \cap H_0^1(\Omega)$ and $w = \kappa\Delta u - \sigma u$. Let $(\tilde{u}, \tilde{w})$ be the unique solution of Problem 2.4.1. By the forwards implication and uniqueness for Problem 2.3.1 it follows $\tilde{u} = u$. Furthermore

$$\tilde{w} = \kappa\Delta\tilde{u} - \sigma\tilde{u} = \kappa\Delta u - \sigma u = w.$$

□

We can solve this reformulated problem numerically using a finite element method. Taking a polygonal approximation of the boundary and a triangulation T_h of the resulting domain Ω_h we produce the usual P^1 finite element space, with zero boundary condition,

$$V_h = \left\{ v_h \in C^0(\overline{\Omega_h}) \mid v_h|_K \in P^1(K) \, \forall K \in T_h \text{ and } v_h|_{\partial\Omega_h} = 0 \right\}.$$

We will assume $\Omega_h \subset \Omega$ throughout this section. Note that it is always possible to construct such Ω_h when Ω is convex. The finite element approximation of our problem may then be stated as follows.

Find u_h, $w_h \in V_h$ such that $\forall v_h \in V_h$:

$$\int_{\Omega_h} \nabla w_h \cdot \nabla v_h = -\sum_{k=1}^{N} \beta_k v_k(X_k),$$
$$\int_{\Omega_h} \kappa \nabla u_h \cdot \nabla v_h + \sigma u_h v_h = -\int_{\Omega_h} w_h v_h.$$

Denote a basis of V_h by $\left\{ \phi_1^h, ..., \phi_{N_h}^h \right\}$. Writing $\mathbf{u} := (u_1, ..., u_{N_h})$ and $\mathbf{w} := (w_1, ..., w_{N_h})$ such that $u_h = \sum_{i=1}^{N_h} u_i \phi_i^h$ and $w_h = \sum_{i=1}^{N_h} w_i \phi_i^h$ we produce an equivalent problem:

Find $\mathbf{u}, \mathbf{w} \in \mathbb{R}^{N_h}$ such that

$$S^h \mathbf{w} = \mathbf{F}^h,$$
$$(\kappa S^h + \sigma M^h)\mathbf{u} + M^h \mathbf{w} = 0.$$

Here M^h and S^h are the usual mass and stiffness matrices given by

$$M_{ij}^h = \int_{\Omega_h} \phi_i^h \phi_j^h \text{ and } S_{ij}^h = \int_{\Omega_h} \nabla \phi_i^h \cdot \nabla \phi_j^h.$$

The right hand side vector is given by

$$F_j^h = -\sum_{k=1}^{N} \beta_k \phi_j^h(X_k).$$

To account for the boundary conditions we identify the basis functions which have support on the boundary and set the corresponding values $u_i, w_i = 0$. To implement this for $\mathbf{w}$ we replace the appropriate rows of S^h by identity rows and the corresponding entries of $\mathbf{F}^h$ are replaced by zeroes. Owing to how we have set up this problem, we solve first for $\mathbf{w}$ and then for $\mathbf{u}$, using $-M^h\mathbf{w}$ as the right hand side in the second equation. We can then implement the boundary condition for $\mathbf{u}$ in the same manner as for $\mathbf{w}$, here we replace appropriate rows in $\kappa S^h + \sigma M^h$ by the identity and entries of $M^h\mathbf{w}$ by zero.

We test this method on the unit circle, $\Omega = B(0,1)$, setting $\kappa = 1$ and $\sigma = 0$ as here the explicit solution is known. This is a linear combination of Green's functions. On the unit circle the Green's function for the bilaplacian with boundary conditions $u = \Delta u = 0$ is given by the following expression, taken from [8],

$$\begin{aligned} G(x,y) = \frac{1}{8\pi}\Bigg[&|y-x|^2 \left(\log|y-x| - \log\sqrt{|x|^2|y|^2 - 2x\cdot y + 1} \right) \\ &- \frac{(1-|x|^2)(1-|y|^2)}{|x|^2|y|^2} \left(x\cdot y \log\sqrt{|x|^2|y|^2 - 2x\cdot y + 1} \right) \\ &+ \frac{(1-|x|^2)(1-|y|^2)}{|x|^2|y|^2} \left((x_1y_0 - x_0y_1)\arctan\left(\frac{x_1y_0 - x_0y_1}{1 - x\cdot y} \right) \right) \Bigg]. \end{aligned} \tag{2.25}$$

Note that $G \in W^{3,s}(B(0,1))$ for any $s \in (1,2)$. The exact solution u is thus given by the expression

$$u(y) = \sum_{k=1}^{N} \beta_k G(X_k, y). \tag{2.26}$$

The exact solution $w = \Delta u$ is hence given by

$$w(y) = \sum_{k=1}^{N} \beta_k \Delta_y G(X_k, y). \tag{2.27}$$

Direct calculation produces the Laplacian term, this is

$$\Delta_y G(X_k, y) = \frac{1}{2\pi}\left[\log|y - X_k| - \log\sqrt{|X_k|^2|y|^2 - 2X_k\cdot y + 1} \right].$$

We now establish the theoretical convergence rates for this method and will compare these with experimental orders of convergence achieved in practice. First we introduce some notation. We will denote the canonical L^2 and H^1 norms by

$$\|u\|_{0,2} := \left(\int_\Omega u^2 \right)^{1/2} \quad \text{and} \quad \|u\|_{1,2} := \left(\int_\Omega |\nabla u|^2 + u^2 \right)^{1/2}.$$

We will also denote the canonical L^2 inner product by

$$(u, v) := \int_\Omega uv.$$

The convergence rates involve comparing discrete functions, elements of V_h, with functions defined on Ω. Note that discrete functions $v_h \in V_h$ are defined on Ω_h rather than Ω. To account for this we extend them by zero in the skin $\Omega \setminus \Omega_h$.

Lemma 2.4.3. *Let $(u_h, w_h) \in V_h \times V_h$ be the solution to the finite element outlined above and (u, w) the exact solution as given in* (2.26) *and* (2.27)*. There exists $C > 0$ such that*

$$\|w - w_h\|_{0,2} + \|u - u_h\|_{1,2} \le Ch \left\| \sum_{k=1}^{N} \beta_k \delta_{X_k} \right\|_{C^0(\Omega)^*}.$$

Finally, if the boundary $\partial\Omega$ is smooth, there exists $C > 0$ such that

$$\|u - u_h\|_{0,2} \le Ch^2 |\log(h)|.$$

Proof. We will assume $N^+ = 1, N^- = 0$ and $\beta_1 = 1$, having shown this case the full result follows by linearity.

Throughout the proof we will denote by $a(\cdot, \cdot)$ the bilinear form

$$a(u, v) := \int_\Omega \kappa \nabla u \cdot \nabla v + \sigma uv.$$

The bound on $\|w - w_h\|_{0,2}$ is proven in [14, 71]. The bound on $\|u - u_h\|_{1,2}$ is then proven as follows. Note $u \in H^2(\Omega)$, $\|u\|_{2,2} \le C\|w\|_{0,2} \le C\|\delta_{X_1^+}\|$ and the P^1 interpolant $I_h u$ is well defined, then

$$\begin{aligned} a(u - u_h, u - u_h) &= a(u - u_h, u - I_h u) + (w - w_h, I_h u - u_h) \\ &\le Ch\|u\|_{2,2}\|u - u_h\|_{1,2} + Ch\|\delta_{X_1^+}\|_{C^0(\Omega)^*} (\|I_h u - u\|_{1,2} + \|u - u_h\|_{1,2}) \\ &\le Ch\|\delta_{X_1^+}\|_{C^0(\Omega)^*}(\|u - u_h\|_{1,2} + h\|\delta_{X_k}\|_{C^0(\Omega)^*}\|). \end{aligned}$$

The $\|u - u_h\|_{1,2}$ bound then follows by applying Young's inequality. Now assume $\partial\Omega$ is smooth. The remaining bound relies upon estimating the error $w - w_h$ in a dual norm, that is

$$\|w - w_h\|_* := \sup \left\{ |(w - w_h, \phi)| \mid \phi \in W_0^{1,q}(\Omega),\ \|\phi\|_{1,q} = 1 \right\},$$

where we fix some $2 < q < \infty$ and $\|\cdot\|_{1,q}$ denotes the $W^{1,q}(\Omega)$ norm. Let $\phi \in W_0^{1,q}(\Omega)$

and $\psi \in H_0^1(\Omega)$ s.t. $(\nabla\psi, \nabla v) = (-\phi, v)\ \forall v \in H_0^1(\Omega)$. By elliptic regularity (recall we now assume $\partial\Omega$ is smooth) $\psi \in W^{3,q} \cap H_0^1(\Omega)$ and $\Delta\psi = \phi$. Finally, let $\psi_h \in V_h$ s.t. $(\nabla\psi_h, \nabla v_h) = (-\phi, v_h)\ \forall v_h \in V_h$, it follows

$$
\begin{aligned}
(w - w_h, \phi) &= (w - w_h, \Delta\psi),\\
&= \psi(X) - \psi_h(X) + (\nabla w_h, \nabla[\psi - \psi_h]),\\
&= \psi(X) - \psi_h(X),\\
&\leq \|\psi - \psi_h\|_{0,\infty},\\
&\leq C|\log(h)| \inf_{v_h \in V_h} \|\psi - v_h\|_{0,\infty},\\
&\leq Ch^2|\log(h)|\|\psi\|_{2,\infty},\\
&\leq Ch^2|\log(h)|\|\psi\|_{3,q},\\
&\leq Ch^2|\log(h)|\|\phi\|_{1,q},\\
\implies \|w - w_h\|_* &\leq Ch^2|\log(h)|.
\end{aligned}
$$

The $|\log(h)|$ bound is given in [68] and the proceeding bound in [15, Theorem 3.1.6].

To produce the L^2 bound, let $\varphi \in V$ be such that $a(\varphi, v) = (u - u_h, v)\ \forall v \in V$ and $\varphi_h \in V_h$ be such that $a(\varphi_h, v_h) = (u - u_h, v_h)\ \forall v_h \in V_h$, it follows

$$
\begin{aligned}
\|u - u_h\|_{0,2}^2 &= a(\varphi - \varphi_h, u - u_h) + a(\varphi_h, u - u_h),\\
&= a(\varphi - \varphi_h, u - u_h) + (w - w_h, \varphi_h),\\
&\leq \|\varphi - \varphi_h\|_{1,2}\|u - u_h\|_{1,2} + \|w - w_h\|_*\|\varphi_h\|_{1,q},\\
&\leq Ch^2\|u\|_{2,2}\|u - u_h\|_{0,2} + Ch^2|\log(h)|\|u - u_h\|_{0,2},
\end{aligned}
$$

from which the L^2 bound is immediate. Note that we use the bound $\|\varphi_h\|_{1,q} \leq C\|u - u_h\|_{0,2}$. Deriving this bound requires use of a discrete inf sup inequality similar to those used in Chapter 5. For brevity the proof of such a bound is not given here, however it may be proven in a similar manner to the similar statements in Chapter 5. $\square$

We note that, as in [71], the constant recovered in the error bound does depend upon the locations of the point forces. Specifically, the constant here will depend upon the distance to the boundary of the point force located nearest the boundary.

The tables below show the errors and experimental orders of convergence on successive refinements for two test problems. The experimental order of convergence is calculated between one refinement and the previous refinement by the formula

$$EOC = \frac{\log(E(h_{n+1})/\log(E(h_n))}{\log(h_{n+1})/\log(h)}.$$

Test Problem 1 : $N = 1, \beta_1 = 1, X_1 = (0, 0)$.

h_n	$E_{L^2(\Gamma)}(h_n)$	EOC	$E_{H^1(\Gamma)}(h_n)$	EOC
2^0	3.87217×10^{-3}	-	2.02112×10^{-2}	-
2^{-1}	1.02684×10^{-3}	1.91493	1.47398×10^{-2}	0.455436
2^{-2}	2.5571×10^{-4}	2.00563	8.02377×10^{-3}	0.877366
2^{-3}	7.8584×10^{-5}	1.7022	4.10184×10^{-3}	0.968009
2^{-4}	2.64382×10^{-5}	1.57161	2.06288×10^{-3}	0.991612
2^{-5}	8.67054×10^{-6}	1.60843	1.03296×10^{-3}	0.997871
2^{-6}	2.72379×10^{-6}	1.67051	5.16667×10^{-4}	0.999481
2^{-7}	8.25134×10^{-7}	1.72291	2.58355×10^{-4}	0.999879
2^{-8}	2.43052×10^{-7}	1.76336	1.2918×10^{-4}	0.999973

Table 2.1: Errors and Experimental orders of convergence for $u_h - u$.

h_n	$E_{L^2(\Gamma)}(h_n)$	EOC
2^0	4.77648×10^{-2}	-
2^{-1}	2.4255×10^{-2}	0.977662
2^{-2}	1.20906×10^{-2}	1.0044
2^{-3}	6.03314×10^{-3}	1.0029
2^{-4}	3.01523×10^{-3}	1.00064
2^{-5}	1.50749×10^{-3}	1.00012
2^{-6}	7.53736×10^{-4}	1.00002
2^{-7}	3.76868×10^{-4}	1.00000
2^{-8}	1.88434×10^{-4}	0.999999

Table 2.2: Errors and Experimental orders of convergence for $w_h - w$.

The numerical method clearly achieves the theoretical order of convergence in practice for the $\|u - u_h\|_{1,2}$ and $\|w - w_h\|_{0,2}$ errors. For the $\|u - u_h\|_{0,2}$ the theoretical rate is $h^2|\log(h)|$ which is harder to verify but our results are certainly consistent with this rate.

Test Problem 2 : $N = 2, \beta_1 = 1, \beta_2 = -1, X_1 = (-0.5, 0), X_2 = (\sqrt{2}/4, \sqrt{2}/4)$.

h_n	$E_{L^2(\Gamma)}(h_n)$	EOC	$E_{H^1(\Gamma)}(h_n)$	EOC
2^0	1.01269×10^{-2}	-	3.9471×10^{-2}	-
2^{-1}	2.63855×10^{-3}	1.94038	1.77138×10^{-2}	1.15592
2^{-2}	8.02705×10^{-4}	1.7168	1.01108×10^{-2}	0.808973
2^{-3}	2.1383×10^{-4}	1.9084	5.25126×10^{-3}	0.945165
2^{-4}	5.48452×10^{-5}	1.96303	2.65579×10^{-3}	0.983526
2^{-5}	1.39107×10^{-5}	1.97917	1.3324×10^{-3}	0.995111
2^{-6}	3.51691×10^{-6}	1.98381	6.66856×10^{-4}	0.998581
2^{-7}	8.88411×10^{-7}	1.98501	3.33521×10^{-4}	0.999597
2^{-8}	2.24392×10^{-7}	1.98521	1.66774×10^{-4}	0.999887

Table 2.3: Errors and Experimental orders of convergence for $u_h - u$.

h_n	$E_{L^2(\Gamma)}(h_n)$	EOC
2^0	1.83815×10^{-1}	-
2^{-1}	3.36504×10^{-2}	2.44956
2^{-2}	1.6958×10^{-2}	0.988658
2^{-3}	8.4926×10^{-3}	0.997687
2^{-4}	4.24875×10^{-3}	0.999167
2^{-5}	2.1248×10^{-3}	0.999715
2^{-6}	1.06247×10^{-3}	0.9999
2^{-7}	5.31249×10^{-4}	0.999966
2^{-8}	2.65626×10^{-4}	0.999988

Table 2.4: Errors and Experimental orders of convergence for $w_h - w$.

In producing these test problems it was observed that the performance of the method depends upon the location of the point forces with respect to the mesh. The optimal convergence rates observed here were obtained when the point forces are located on nodes of the mesh, that is on vertices of triangles rather than in their interior.

2.4.2 Numerical results

Recall that we are considering Problem 2.3.1 with point forces at fixed locations $X = (X_i) \in \overline{\Omega}$ and the solution space $V = H^2(\Omega) \cap H_0^1(\Omega)$. We wish to study the membrane-mediated interactions between point forces and produce an energy profile as we vary the locations of forces within the domain Ω. We have shown that point forces of equal sign cluster to one point (see Corollary 2.3.1). Thus, we restrict the investigation of membrane-mediated interactions to the case $N = 2$ and $\alpha_1 < 0 < \alpha_2$. Precisely, we choose $\alpha_1 = -10$, $\alpha_2 = 10$, $\kappa = 1$ and the domain $\Omega = \{x \in \mathbb{R}^2 \mid |x| < 1\}$ for all subsequent computations. To study the interaction potential between the two opposite forces, we fix $X_1 = (0, 0)$, allow X_2 to vary along the abscissa and compute the resulting approximate minimal energy $\mathcal{J}$ as a function of the separation distance R. This is done for a variety of values of σ.

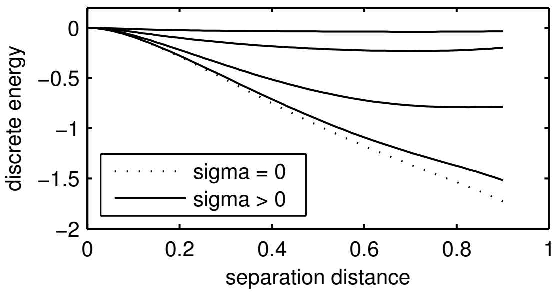
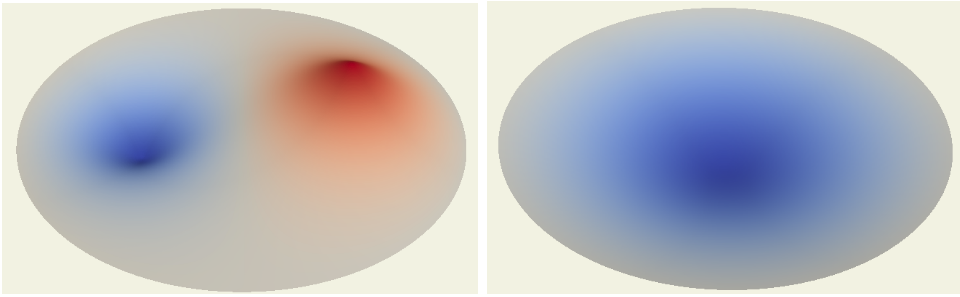


Figure 2.4: Interaction potential for opposite point forces over separation distance for $\sigma = 0, 1, 10, 100, 1000$ (bottom up).

The results depicted in Figure 2.4 show that opposite forces repel each other and that this repulsion depends upon the ratio κ/σ. Increasing σ, i.e. decreasing the ratio κ/σ, yields a decrease in the distance over which the repulsive interaction plays a role. For $\sigma = 1$ the repulsion persists close to the boundary, whereas for higher values of σ the repulsion has a shorter length scale and is, from a certain distance R^* on, dominated by the inwards force applied at the boundary. Note that this inwards force is a consequence of the (artificial) boundary condition $u = 0$.

Discussion

The above numerical findings could be related to the theoretical results derived in Section 2.3.2. According to Remark 2.3.1, there are essentially two types of global minimizers solving Problem 2.3.2. A type 1 global minimizer is characterised by X^+,



(a) type 1 global minimizer (b) type 2 global minimizer

Figure 2.5: Approximate membrane displacement for different types of global energy minimizers.

$X^- \in \Omega$ (case (i)) and type 2 means that either X^+ or X^- is located on $\partial\Omega$ (cases (ii) and (iii)). The numerical results shown in Figure 2.4 indicate that type 1 or type 2 minimizers occur for sufficiently small or large ratio κ/σ, respectively. Figure 2.5a shows a type 1 global minimizer solving Problem 2.3.2 for $\kappa = \sigma = 1$ while Figure 2.5b illustrates a type 2 global minimizer occurring for $\kappa = 1$, $\sigma = 100$. Recall that type 2 global minimizers only occur due to influence of the domain boundary. Thus, it is not surprising that there is no such result in the existing literature that mostly concentrates on unbounded asymptotically flat membranes. However, dependence of the length scale of repulsive interactions between particles which apply forces to the membrane upon the ratio κ/σ is well known and discussed, e.g., in [33]. One could work on estimating biologically relevant values for the parameters used here but the results would be qualitatively no different to what we have observed. The problem is linear in the magnitudes of the point forces and as long the ratio κ/σ is fixed, changing these parameters is simply a rescaling of the problem. Typical ranges for $\sqrt{\kappa/\sigma}$ are between $6nm$ and $100nm$, see [33], thus in our experiments we have varied the ratio κ/σ by four orders of magnitude. Even if the biologically relevant regime lies outside of the range chosen here we have still captured the qualitative behaviour of the system.

Finally note that we have only dealt with point forces in our numerical experiments. However, one could employ this technique to approximate solutions to the point constraints problems via a penalty method, utilizing general results stated in Proposition A.2.1. Such a problem could be treated in complete analogy to soft point curvature constraints which will be studied in the next chapter.

Chapter 3

Eighth order problems on a planar membrane

3.1 Augmented Canham-Helfrich free energy

3.1.1 Point approximation of mean values

We will now consider fixing the curvature of the membrane at particular points. This models a different type of interaction with the membrane than was studied in the previous chapter. Now we are concerned with particles, often termed inclusions, which are embedded into the membrane or lie on it and locally fix its shape. These can be modelled in the same regime we used previously, that is the Monge gauge and using the linearised Canham-Helfrich energy (2.7). To do so one considers the reference domain

$$\Omega_B := \Omega \setminus \bigcup_{i=1}^{N} \overline{B_i},$$

where the set B_i, for $i = 1, ..., N$, represents the cross section of particle i. The deformation effect is encoded in prescribing boundary conditions along ∂B_i. This is discussed at length in [31]. There this model is linked with with the point model that will be used here through averaged constraints, using the functionals

$$f_i(v) = \fint_{\partial B_i} v \, ds, \qquad g_i(v) = \fint_{\partial B_i} \frac{\partial}{\partial n} v \, ds, \qquad i = 1, \dots, N, \tag{3.1}$$

where $\fint_D := \frac{1}{|D|} \int_D$. Notice that the g_i terms can be rewritten by utilizing Green's formula, the functionals g_i, $i = 1, \dots, N$, can be expressed as averaged mean curvature according to

$$g_i(v) = -\frac{|B_i|}{|\partial B_i|} \fint_{B_i} \Delta v \, dx, \qquad v \in V, \tag{3.2}$$

where the sign results from the fact that n is an inward normal to B_i.

When the particles are circular and have a small diameter with respect to the diameter of the domain then it is of interest to consider modelling the particles as points. One approach to obtaining such models is to replace integrals by point evaluations. That is, the mean value $\fint_{B_i} \Delta u \, dx$ is naturally approximated by $\Delta u(X_i)$ by sending the diameter of the ball B_i to zero. This may be understood in a different way as approximating the integrals in the averages (3.1) by a first-order Gauss formula. Constraints on the functionals g_i then take the form

$$Gu = \left(\tfrac{-|\partial B_i|}{|B_i|} \bar{s}_i \right) \tag{3.3}$$

with $G = (G_i)$, and functionals G_i defined by

$$G_i u = \delta_{X_i}(\Delta u), \qquad i = 1, \dots, N, \tag{3.4}$$

and given $\bar{s}_i \in \mathbb{R}$ according to

$$\bar{s}_i := \fint_{\partial B_i} s_i \, ds$$

where $s_i \in H^{1/2}(\partial B_i)$ is the $\partial u / \partial n$ boundary condition imposed by the particle B_i. Here,

$$\delta_x v = v(x), \qquad x \in \overline{\Omega},$$

denotes the Dirac functional.

3.1.2 Well posedness

Due to the continuous embedding $H^2(\Omega) \subset C(\overline{\Omega})$ (see, e.g., [1, Theorem 4.12]), the Dirac functional δ_x is a bounded linear functional on $H^2(\Omega)$. However, the functionals G_i are not well-defined on $v \in H^2(\Omega)$, because the linearised mean curvature $\Delta v \in L^2(\Omega)$ in general does not allow for point values. In order to state a well-posed minimization problem on a smaller solution space of sufficiently regular functions, we augment the Canham-Helfrich energy $\mathcal{J}$ defined in (2.7) by additional higher order terms to obtain

$$\tilde{\mathcal{J}}(u) = \mathcal{J}(u) + \int_\Omega \tfrac{\kappa_8}{2}|\Delta^2 u|^2 + \tfrac{\kappa_6}{2}|\nabla\Delta u|^2 \, dx, \qquad u \in H^4(\Omega), \tag{3.5}$$

with some given regularization parameters κ_8, $\kappa_6 > 0$. This artificial extension could be replaced by a more realistic fourth-order expansion of the bending energy with respect to principal curvatures [46, 57].

The strict positivity of κ_8 guarantees that functions which have bounded energy lie in $H^4(\Omega)$. In turn, the continuous embedding $H^4(\Omega) \subset C^2(\overline{\Omega})$ implies that the $G_i = \delta_{X_i}(\Delta\,\cdot)$ are bounded linear functionals on $H^4(\Omega)$. Note that the functionals G_i are linearly independent for distinct locations X_i, $i = 1, \dots, N$. This also holds for point values of second-order derivatives $\delta_{X_i}(\partial_{xx}\,\cdot)$, $\delta_{X_i}(\partial_{xy}\,\cdot)$, and $\delta_{X_i}(\partial_{yy}\,\cdot)$.

Differentiation of $\tilde{\mathcal{J}}$ yields the associated bilinear form

$$\tilde{a}(u,v) = \int_\Omega \kappa_8 \Delta^2 u \Delta^2 v + \kappa_6 \nabla\Delta u \cdot \nabla\Delta v + \kappa \Delta u \Delta v + \sigma \nabla u \cdot \nabla v. \tag{3.6}$$

The higher order terms in $\tilde{\mathcal{J}}$ give rise to additional boundary conditions defining a suitable closed solution space $\tilde{V} \subset H^4(\Omega)$. For example, we might choose

$$\tilde{V} = \begin{cases} H^4(\Omega) \cap H^3_0(\Omega) = \{v \in H^4(\Omega) \mid v = \frac{\partial}{\partial n} v = \frac{\partial^2}{\partial n^2} v = 0 \text{ on } \partial\Omega\}, \\ \{v \in H^4(\Omega) \mid v = 0,\ \Delta v = 0 \text{ on } \partial\Omega\}, \\ H^4_{p,0}(\Omega) = \overline{\{v|_\Omega \mid v \in C^\infty(\mathbb{R}^2) \text{ is } \Omega\text{-periodic and } \int_\Omega v \, ds = 0\}}. \end{cases}$$

For the final two cases we consider only rectangular domains Ω. Each choice for $\tilde{V}$ also provides complementary natural boundary conditions for solutions to variational problems posed in that space. Observe that $\tilde{a}(\,\cdot\,,\,\cdot\,)$ is bounded and symmetric on $\tilde{V}$. It is also coercive for any $\kappa_8 > 0$ and κ_6, κ, $\sigma \geq 0$, see Appendix B.

3.2 Point curvature constraints

3.2.1 Fixed locations of particles

We first consider imposing the point curvature constraints at fixed locations within the domain Ω.

Problem 3.2.1 (Point mean curvature constraints)**.**
Find $u \in \tilde{V}$ minimizing the energy $\tilde{\mathcal{J}}(u)$ on $\tilde{V}$ subject to the constraints (3.3).

Proposition 3.2.1. *There exists a unique solution $u \in \tilde{V}$ to Problem 3.2.1.*

Proof. The particles B_i are disjoint, so that we have $X_i \neq X_j$, for $i \neq j = 1, \ldots, N$. Hence, the functionals G_i are linearly independent. Now the assertion follows from Proposition A.1.1 in the appendix. □

Possible anisotropies can be represented by the geometry of particles B_i and boundary conditions they impose. These are lost completely in the approximation by point mean curvature constraints. Accounting for anisotropies we now prescribe different curvatures

$$G_{i,1}u = \delta_{X_i}(\partial_{xx}u), \quad G_{i,2}u = \delta_{X_i}(\partial_{xy}u), \quad G_{i,3}u = \delta_{X_i}(\partial_{yy}u) \tag{3.7}$$

at one point X_i for $i = 1, \ldots, N$. We set $G = (G_{i,j}) \in (\tilde{V}')^{N\times 3}$.

Problem 3.2.2 (Point curvature constraints)**.**
Find $u \in \tilde{V}$ minimizing the energy $\tilde{\mathcal{J}}(u)$ on $\tilde{V}$ subject to the constraints

$$G(u) = r \tag{3.8}$$

with given $r = (r_{i,j}) \in \mathbb{R}^{N\times 3}$.

The functionals $G_{i,j}$ defined in (3.7) are linearly independent for distinct locations X_i. Hence, existence and uniqueness again follows from Proposition A.1.1.

Proposition 3.2.2. *There exists a unique solution $u \in \tilde{V}$ to Problem 3.2.2.*

We now derive an explicit representation of u in terms of Green's functions $\phi_{i,j} \in \tilde{V}$, which are defined as the unique solutions of the variational problems

$$\tilde{a}(\phi_{i,j}, v) = G_{i,j}v \qquad \forall v \in \tilde{V}, \quad i = 1, \ldots, N, \quad j = 1, 2, 3. \tag{3.9}$$

As each $G_{i,j}$ is a bounded linear functional on $H^4(\Omega)$ existence and uniqueness of the above Green's functions follows from the Lax-Milgram theorem.

Proposition 3.2.3. *Let $A = (\tilde{a}(\phi_{i,j}, \phi_{k,l})) \in \mathbb{R}^{(N\times 3)\times(N\times 3)}$. Then*

$$u = \sum_{i=1}^{N}\sum_{j=1}^{3} u_{i,j}\phi_{i,j} \tag{3.10}$$

holds with $(u_{i,j}) = A^{-1}r \in \mathbb{R}^{N\times 3}$.

Proof. The assertion follows from the abstract Proposition A.1.1 as applied to the special case $\ell = 0$ and thus $\phi_0 = 0$. □

We now consider *soft curvature constraints*. To this end we augment the energy $\tilde{\mathcal{J}}$ by the penalty term

$$\frac{1}{2\varepsilon}\|Gu - r\|^2_{\mathbb{R}^{N\times 3}} \tag{3.11}$$

with some small penalty parameter $\varepsilon > 0$ and the Frobenius norm $\|\cdot\|_{\mathbb{R}^{N\times 3}}$. There are two reasons for our interest in soft curvature constraints. Mathematically we will use such problems to approximate the hard constraints problem as the penalty method is easier to implement a finite element method for. Physically, the soft constraints may be interpreted as a basic model for the interplay between the membrane and the protein inclusions. The membrane is under tension and thus applies a force to inclusions which may deform them, depending upon their rigidity. We may incorporate this by modelling more rigid inclusions with smaller values of ε.

Problem 3.2.3 (Soft point curvature constraints)**.**
Find $u_\varepsilon \in \tilde{V}$ minimizing the energy

$$\tilde{\mathcal{J}}(u_\varepsilon) + \frac{1}{2\varepsilon}\|Gu_\varepsilon - r\|^2_{\mathbb{R}^{N\times 3}}$$

on $\tilde{V}$.

While existence and uniqueness follows from the Lax-Milgram lemma, Proposition A.2.1 implies convergence to the hard-constrained solution.

Proposition 3.2.4. *Let u denote the solution of Problem 3.2.2 and u_ε denote the solution of Problem 3.2.3 for fixed $\varepsilon > 0$. Then we have*

$$u_\varepsilon \to u \quad \text{in } \tilde{V} \qquad \text{as} \quad \varepsilon \to 0.$$

Remark 3.2.1. *The results stated in Proposition 3.2.3 and 3.2.4 also hold literally for $G = (G_i) \in (\tilde{V}')^N$ with functionals G_i defined in* (3.4).

3.2.2 Varying the locations of particles

We now seek a global minimizer over prescribed curvatures in the sense that we allow for varying locations $X = (X_i)$ of particles. To emphasize that the functionals

$G = (G_{i,j})$ defined in (3.7) depend on the locations X_i, we introduce the notation

$$G_X = (G_{X,i,j}) \in (\tilde{V}')^{N\times 3} \qquad G_{X,i} \in (\tilde{V}')^3. \tag{3.12}$$

First we consider hard-wall constraints, i.e., we restrict the locations X to a subset ω so that the particles would not overlap with each other or the boundary. Precisely, the set $\omega \subset \Omega^N$ is given by

$$\omega = \{X \in \Omega^N \mid B(X_i) \cap B(X_j) = B(X_i) \cap \partial\Omega = \emptyset \ \forall i \neq j\}.$$

Here $B(X_i)$ denotes the open ball centred at X_i with some fixed radius R which models the physical diameter of the particles. The set ω is compact, evidently it is bounded and it is closed as if $X^n \to X$ then the minimal separation of points X_i from each other and the boundary passes to the limit. For a full proof see [31, Lemma 6].

Problem 3.2.4 (Point curvature constraints with varying locations)**.**
Find $(u, X) \in \tilde{V} \times \omega$ *minimizing the energy* $\tilde{\mathcal{J}}(u)$ *on* $\tilde{V}$ *subject to the constraint that there is an* $X = (X_i) \in \omega$ *such that*

$$G_X u = r$$

holds with given $r \in \mathbb{R}^{N\times 3}$.

Lemma 3.2.1. *For any* $X \in \omega$ *the family* $(G_{X,i,j}) \in (\tilde{V}')^{N\times 3}$ *of functionals* $G_{X,i,j} \in \tilde{V}'$ *is linearly independent and* $G_X : \tilde{V} \to \mathbb{R}^{N\times 3}$ *is surjective.*

Proof. Let $X \in \omega$. First we note that surjectivity of $G_X : \tilde{V} \to \mathbb{R}^{N\times 3}$ is equivalent to linear independence of the family $(G_{X,i,j})$. Evidently $X_i \in B(X_i)$ and hence, by the definition of ω, $X_i \neq X_j$ for $i \neq j$. Hence we can construct smooth functions v with $G_X v = r$ for any $r \in \mathbb{R}^{N\times 3}$. □

Proposition 3.2.5. *Assume that* $\omega \neq \emptyset$*. Then there exists a solution* $(u, X) \in \tilde{V} \times \omega$ *to Problem 3.2.4.*

Proof. In order to apply Proposition A.1.2, we first note that, by Lemma 3.2.1, for any $Y \in \omega$ there is a $v \in \tilde{V}$ with $G_Y v = r$, i.e., the feasible set is non-empty.

It remains to show that the mapping $\omega \ni X \to G_X \in (\tilde{V}')^{N\times 3}$ is continuous on the compact set ω (cf. [31, Lemma 6]). To this end let $X, Y \in \omega$, $v \in \tilde{V}$, $i \in \{1, \ldots, N\}$, and, without loss of generality, $j = 1$. Since the Sobolev embedding theorem provides $\tilde{V} \subset H^4(\Omega) \to C^{2,\lambda}(\overline{\Omega})$ for any Hölder-exponent $0 < \lambda < 1$ (see, e.g., [1, Theorem 4.12]), we have

$$|(G_X - G_Y)_{i,j}v| = |\partial_{xx}v(X_i) - \partial_{xx}v(Y_i)| \leq \|v\|_{C^{2,\lambda}}|X_i - Y_i|^\lambda \leq C\|v\||X_i - Y_i|^\lambda$$

and thus $\|G_X - G_Y\|_{(\tilde{V}')^{N\times 3}} \to 0$ as $X \to Y$. This concludes the proof. $\square$

We now provide a reformulation of Problem 3.2.4 in terms of suitable Green's functions.

Proposition 3.2.6. *Assume that $\omega \neq \emptyset$. For given $Y \in \omega$, let the Green's functions $\phi_{Y,i,j} \in \tilde{V}$ and the matrix $A_Y = \tilde{a}(\phi_{Y,i,j}, \phi_{Y,k,l}) \in \mathbb{R}^{(N\times 3)\times(N\times 3)}$ be defined as in* (3.9) *and Proposition 3.2.3, respectively. Then each solution (u, X) of Problem 3.2.4 has the representation*

$$u = \sum_{i=1}^{N}\sum_{j=1}^{3} u_{i,j}\phi_{X,i,j}, \quad (u_{i,j}) = A_X^{-1}r \tag{3.13}$$

where X is a minimizer of the mapping

$$\omega \ni Y \mapsto r^\top A_Y^{-1}r \in \mathbb{R}.$$

Proof. Note that Lemma 3.2.1 implies that the family $(G_{Y,i,j})$ is linearly independent for all $Y \in \omega$. Hence Proposition A.1.3 can be applied for the special case $\ell = 0$ (and thus $\phi_0 = 0$). $\square$

Now we consider soft-wall constraints by augmenting the energy functional with the term $\mathcal{V}_{\text{soft}}(X)$. Denoting $B(X_i)$ by B_i, this term takes the form $\mathcal{V}_{\text{soft}} = \mathcal{V}_1 + \mathcal{V}_2$ consisting of a Lennard-Jones potential

$$\mathcal{V}_1(X) = \sum_{\substack{i,j=1\\ i\neq j}}^{N} \mathcal{V}_{ij}, \quad \mathcal{V}_{ij} = 4\epsilon_{ij}\left[\left(\frac{\sigma_{ij}}{\operatorname{dist}(B_i, B_j)}\right)^{12} - \left(\frac{\sigma_{ij}}{\operatorname{dist}(B_i, B_j)}\right)^{6}\right], \tag{3.14}$$

for $X \in \omega$ such that $\operatorname{dist}(B_i, B_j) > 0$, $i \neq j$ and $\mathcal{V}_1(X) = \infty$ otherwise.

This term accounts for the repulsion and attraction of particles, a typical potential is plotted in Figure 3.1. The values $\sigma_{ij} > 0$ can be used to tune the location of the minimum. The potential is primarily used to ensure that particles do not overlap as this is not physically possible. However one could use a similar potential to account for non membrane-mediated interactions between particles which may

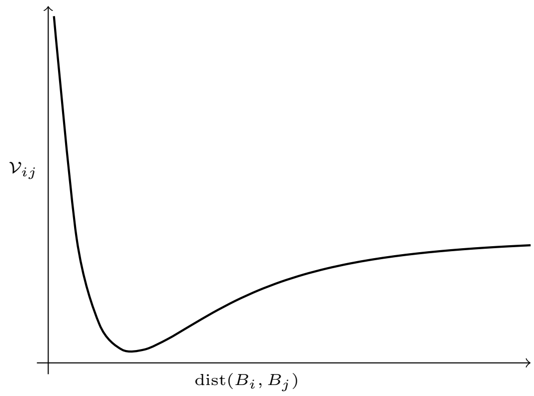


Figure 3.1: A typical Lennard-Jones potential

occur in some physical examples. The long range attraction is also physical, see for example [24].

We also define

$$\mathcal{V}_2(X) = \sum_{i=1}^{N} \left(\frac{\sigma_i}{\mathrm{dist}(B_i, \partial\Omega)} \right)^6, \tag{3.15}$$

for $X \in \omega$ such that $\mathrm{dist}(B_i, \partial\Omega) > 0$, $i = 1, \ldots, N$, and $\mathcal{V}_2(X) = \infty$ otherwise. This term is accounting for escaping particles. For circular particles we have $\mathrm{dist}(B_i, B_j) = |X_i - X_j| - 2R$. Note that the soft-wall potential $\mathcal{V}_{\mathrm{soft}} = \mathcal{V}_1 + \mathcal{V}_2$ is continuously differentiable on $\mathrm{int}\,\omega$.

Problem 3.2.5 (Point curvature constraints with varying locations and soft-wall constraints)**.**
Find $(u, X) \in \tilde{V} \times \mathrm{int}\,\omega$ minimizing the energy $\tilde{\mathcal{J}}(u) + \mathcal{V}_{soft}(X)$ subject to the constraint

$$G_X u = r$$

for given $r \in \mathbb{R}^{N\times 3}$.

Proposition 3.2.7. *Assume that $\mathrm{int}\,\omega \neq \emptyset$. Then there exists a solution $(u, X) \in \tilde{V} \times \mathrm{int}\,\omega$ to Problem 3.2.5.*

Proof. Noting that $\mathcal{V}_{\mathrm{soft}}(Y) < \infty$ for all $Y \in \mathrm{int}\,\omega$, we can prove existence of solutions $(u, X) \in \tilde{V} \times \omega$ as in the proof of Proposition 3.2.5. Then $X \in \mathrm{int}\,\omega$ follows from the definition of $\mathcal{V}_{\mathrm{soft}}$. □

Proposition 3.2.8. *Assume that $\omega \neq \emptyset$. Then for each solution (u, X) of Problem 3.2.5 we can represent u as in Proposition 3.2.6 where where X is now a minimizer of the mapping*

$$\omega \ni Y \mapsto r^\top A_Y^{-1} r + \mathcal{V}_{soft}(Y) \in \mathbb{R}.$$

Proof. The proof can be carried out literally as for Proposition 3.2.6. $\square$

Remark 3.2.2. *The results stated in the Propositions 3.2.5, 3.2.6, 3.2.7, and 3.2.8 also hold for $G_X = (G_{X,i}) \in (\tilde{V}')^N$ with functionals $G_{X,i} = \delta_{X_i}(\Delta\,\cdot)$ defined according to* (3.4).

3.2.3 Unbounded domains

In the preceding sections, we have focussed on problems with particles on a membrane that is parametrized over a bounded domain $\Omega \subset \mathbb{R}^2$. However, our variational approach is not limited to this case. As an example, we will now consider a physical model as suggested by [4] with an unbounded membrane parametrized over $\mathbb{R}^2$. We will formulate this model in terms of our variational framework and then use our general theory to recover some, but not all results that were obtained for bounded domains.

Hard and soft point constraints in $\mathbb{R}^2$

Following [4], we consider an extension

$$F_m(u) = \tilde{\mathcal{J}}(u) + \boldsymbol{\gamma} \int_{\mathbb{R}^2} u^2 \, dx, \qquad u \in H^4(\mathbb{R}^2), \tag{3.16}$$

of the energy functional $\tilde{\mathcal{J}}$ defined in (3.5), where Ω is replaced by $\mathbb{R}^2$, by an additional confining potential $\boldsymbol{\gamma} u^2$ with a given constant $\boldsymbol{\gamma} > 0$. The confining potential is required to ensure the resulting minimisation problems are well posed as there is no longer a boundary to our domain.

The coupling of the membrane with N pointwise isotropic particles at pairwise distinct locations $X_i \in \mathbb{R}^2$ is represented by the interaction term

$$\frac{\boldsymbol{\Gamma}}{2} \sum_{i=1}^{N} (G_{X,i} u - C_i)^\top \mathbf{N} (G_{X,i} u - C_i) \tag{3.17}$$

with the 3×3 matrix

$$\mathbf{N} = \begin{pmatrix} 1+\epsilon & 0 & \epsilon \\ 0 & 2 & 0 \\ \epsilon & 0 & 1+\epsilon \end{pmatrix}, \tag{3.18}$$

the Dirac functionals $G_{X,i,j}$ defined in (3.12), $i = 1, \ldots, N$, and given data $C = (C_{i,j}) \in \mathbb{R}^{N\times 3}$, $\mathbf{\Gamma} \geq 0$, and $\epsilon > -1/2$, such that $\mathbf{N}$ is symmetric positive definite. Now the model considered by Bartolo and Fournier [4] reads as follows.

Problem 3.2.6 (Soft point curvature constraints in $\mathbb{R}^2$)**.**
Find $u \in H^4(\mathbb{R}^2)$ minimizing the energy

$$F_m(u) + \frac{\mathbf{\Gamma}}{2} \sum_{i=1}^{N} (G_{X_i} u - C_i)^\top \mathbf{N} (G_{X_i} u - C_i). \tag{3.19}$$

Proposition 3.2.9. *There exists a unique solution to Problem 3.2.6.*

Proof. First we note that the bilinear form

$$a_m(u,v) = \tilde{a}(u,v) + \boldsymbol{\gamma} \int_{\mathbb{R}^2} uv \, dx \tag{3.20}$$

associated with the energy functional F_m is bounded on $H^4(\mathbb{R}^2)$. By partial integration (to account for the mixed derivative terms appearing in the H^4 norm) and the fact that the C^∞-functions with compact support are dense $a_m(\cdot\,,\cdot)$ is also coercive on this space. Furthermore the Sobolev embedding $H^4(\mathbb{R}^2) \to C^2(\mathbb{R}^2)$ (see, e.g., [1, Theorem 4.12]), guarantees continuity of each $G_{X,i,j}$. Since $\mathbf{N}$ is symmetric and positive definite for $\epsilon > -1/2$ this implies that the bilinear form

$$a_m(u,v) + \frac{\mathbf{\Gamma}}{2} \sum_{i=1}^{N} (G_{X,i} u)^\top \mathbf{N} (G_{X,i} v)$$

associated with the energy functional in (3.19) is symmetric and $H^4(\mathbb{R}^2)$-elliptic. Hence, the assertion follows from the Lax-Milgram lemma. $\square$

In order to identify the hard constrained version of Problem 3.2.6, we reformulate the interaction term defined in (3.17) according to

$$\frac{\mathbf{\Gamma}}{2} \sum_{i=1}^{N} (G_{X,i} u - C_i)^\top \mathbf{N} (G_{X,i} u - C_i) = \frac{\mathbf{\Gamma}}{2} \sum_{i=1}^{N} |Q(G_{X,i} u - C_i)|^2, \tag{3.21}$$

where $Q = \mathbf{N}^{\frac{1}{2}} \in \mathbb{R}^{3\times 3}$. For increasing penalty parameter $\mathbf{\Gamma} \to \infty$, we therefore obtain the following hard-constrained problem.

Problem 3.2.7 (Point curvature constraints in $\mathbb{R}^2$)**.**
Find $u \in H^4(\mathbb{R}^2)$ minimizing the energy $F_m(u)$ subject to the constraints

$$G_X u = C. \tag{3.22}$$

Proposition 3.2.10. *There exists a unique solution $u \in H^4(\mathbb{R}^2)$ to Problem 3.2.7. Moreover, denoting the solution of Problem 3.2.6 for fixed $\mathbf{\Gamma} \geq 0$ by $u_{\mathbf{\Gamma}}$, we have*

$$u_{\mathbf{\Gamma}} \to u \quad in \quad H^4(\mathbb{R}^2) \quad for \quad \mathbf{\Gamma} \to \infty. \tag{3.23}$$

Proof. First recall that the bilinear form $\tilde{a}(u, v)+\gamma \int_{\mathbb{R}^2} uv\, dx$ is bounded, symmetric, and coercive on $H^4(\mathbb{R}^2)$ and that the operator G_X is bounded. Furthermore by Lemma 3.2.1 the functionals $G_{X,i,j}$ are linearly independent for pairwise distinct locations X_i. Hence existence and uniqueness follows from Proposition A.1.1.

Finally, since Q is regular, the constraint (3.22) is equivalent to

$$Q(G_{X,i}u - C_i) = 0, \quad i = 1, \dots, N$$

such that the convergence (3.23) is a consequence of Proposition A.2.1. □

We now derive a hard constrained limit version of the stationary energy equation (14) in [4], in our notation this equation reads

$$F_{\text{tot,min}} = \frac{1}{2}\sum_{i=1}^{2} \kappa(C_1, C_2)^T \left(\mathbf{M} + \frac{\kappa}{\mathbf{\Gamma}}\mathbf{N} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\right)^{-1} (C_1, C_2)$$

where $\mathbf{M}$ is as given in [4], we will relate this to our notation shortly. Since we would like to emphasize the dependence of this energy on the locations $X = (X_i)$, $X_i \in \mathbb{R}^2$, we will denote the solution of Problem 3.2.7 for fixed X by u_X from now on. Then Proposition A.1.1 provides the representation

$$u_X = \sum_{i=1}^{N}\sum_{j=1}^{3} u_{X,i,j}\phi_{X,i,j}, \qquad (u_{X,i,j}) = A_X^{-1}C \in \mathbb{R}^{N\times 3}$$

with Green's functions $\phi_{X,i,j}$ and the matrix $A_X \in \mathbb{R}^{(N\times 3)\times(N\times 3)}$ given by

$$a_m(\phi_{X,i,j}, v) = G_{X,i,j}(v) \quad \forall v \in H^4(\mathbb{R}^2) \tag{3.24}$$

and $A_X = (a_m(\phi_{X,i,j}, \phi_{X,k,l}))$, respectively. Lemma A.1.3 implies that the energy at the minimizer is given by

$$F_m(u) = \tfrac{1}{2} C^\top A_X^{-1} C. \tag{3.25}$$

We conclude this section with an explicit representation of the entries of A_X as appearing in [4]. To this end let $\mathcal{G} \in H^4(\mathbb{R}^2)$ denote the Green's function given by

$$a_m(\mathcal{G}, v) = v(0) \qquad \forall v \in H^4(\mathbb{R}^2) \tag{3.26}$$

and define the differential operators $\partial^{(1)} = \partial_{xx}$, $\partial^{(2)} = \partial_{xy}$, and $\partial^{(3)} = \partial_{yy}$. Then $\mathcal{G}$ can be related to the Green's functions $\phi_{X,i,j}$ in the following way.

Lemma 3.2.2. *For $j = 1, 2, 3$ we have $\partial^{(j)}\mathcal{G}(\,\cdot\, - X_i) = \phi_{X,i,j}$.*

Proof. Let $w \in C^\infty(\mathbb{R}^2)$ and set $v = \partial^{(j)} w(\,\cdot\, + X_i) \in C^\infty(\mathbb{R}^2)$. Inserting this in (3.26) gives

$$a_m(\mathcal{G}, v) = v(0) = \partial^{(j)} w(X_i) = G_{X,i,j}(w).$$

By the regularity result given in Lemma C.2.2 in the appendix we have $\mathcal{G} \in H^6(\mathbb{R}^2)$. Hence we have $\partial^{(j)}\mathcal{G} \in H^2(\mathbb{R}^2)$ and partial integration and translation invariance of integrals over $\mathbb{R}^2$ yields

$$a_m(\mathcal{G}, v) = a_m(\mathcal{G}, \partial^{(j)} w(\,\cdot\, + X_i)) = a_m(\partial^{(j)}\mathcal{G}, w(\,\cdot\, + X_i)) = a_m(\partial^{(j)}\mathcal{G}(\,\cdot\, - X_i), w).$$

Since $C^\infty(\mathbb{R}^2)$ is dense in $H^4(\mathbb{R}^2)$ we have shown that $\partial^{(j)}\mathcal{G}(\,\cdot\, - X_i)$ coincides with the unique solution $\phi_{X,i,j}$ of (3.24). $\square$

Now we can insert $\phi_{X,i,j} = \partial^{(j)}\mathcal{G}(\,\cdot\, - X_i)$ into (3.24) to obtain

$$(A_X)_{(i,j),(k,l)} = a_m(\phi_{X,i,j}, \phi_{X,k,l}) = G_{X,i,j}\phi_{X,k,l} = \partial^{(j)}\partial^{(l)}\mathcal{G}(X_k - X_i).$$

Therefore, in the case of $N = 2$ particles, identify $\kappa A_X \in \mathbb{R}^{(2\times 3)\times(2\times 3)}$ with the matrix $\mathbf{M} \in \mathbb{R}^{6\times 6}$ given in equation (8) of [4]. Hence, (3.25) leads to

$$F_m(u_{\mathbf{r}}) = \tfrac{1}{2}\kappa C^\top (\mathbf{M})^{-1} C$$

which precisely agrees with equation (14) in [4] after formally taking the limit $\mathbf{\Gamma} \to \infty$. As a consequence, using the approximation for the matrix $\mathbf{M}$ from [4], our results reproduce the interaction potential for hard constraints denoted by $F_{\text{int,hard}}(r) =$

$F_{\text{int,hard}}(|X_2 - X_1|)$ in equation (20) of [4].

Varying the location of particles

In analogy to Problem 3.2.4 with locations of particles varying in the compact set $\overline{\Omega}$, we now consider varying locations in $\mathbb{R}^2$. We first fix some notation for the $\mathbb{R}^2$ analogue of the set $\omega \subset \overline{\Omega}^N$,

$$\tilde{\omega} = \{X \in \mathbb{R}^{N\times 2} \mid B_i(X) \cap B_j(X) = \emptyset \ \forall i \neq j\}.$$

Recall $G_X = (G_{X,i,j})$ with $G_{X,i,j}$ defined in (3.12) and let $C = (C_{i,j}) \in \mathbb{R}^{N\times 3}$ be given.

Problem 3.2.8 (Point curvature constraints with varying locations in $\mathbb{R}^2$)**.**
Find $(u, X) \in H^4(\mathbb{R}^2) \times \tilde{\omega}$ such that u minimizes the energy $F_m(u)$ subject to the constraint

$$G_X = C. \tag{3.27}$$

Note that Proposition A.1.2 can be no longer applied to prove existence, because $\tilde{\omega}$ is not compact. While we could still show that $\tilde{\omega}$ is closed, it fails to be bounded here. Furthermore, we should not expect a solution to Problem 3.2.8 to exist. To see this, consider the case of $N = 2$ particles at varying locations $X = (X_1, X_2) \in \tilde{\omega}$ and choose $C = (C_1, C_2)$ in such a way that their interaction energy decreases with separation. As an example, one might choose identical isotropic particles as considered, e.g., by Bartolo and Fournier [4]. Let u_X be the unique solution of the corresponding Problem 3.2.7 with fixed locations X. Then $F_m(u_X)$ is precisely the interaction energy and is well-known to strictly decrease as the points X_1 and X_2 are moved apart. As the distance between X_1 and X_2 can become arbitrary large, there can be no minimal set of locations and thus no solution of the corresponding Problem 3.2.8.

3.2.4 Discussion

The constrained minimization Problems 3.2.1 and 3.2.2 stem from the models discussed, e.g., in [4, 23, 24, 48, 53, 60, 61, 80]. See also [36, 63]. The addition of the higher order terms to the energy functional (see (3.5)) to ensure well posedness is done in [4]. Prior to this the ill posedness is dealt with by only studying large separation distances between particles [53] or by truncating the Fourier expansion of the solution, termed the high wave-vector cutoff in [24]. When put in our framework, these papers study an energy functional of the form given in equation (3.19).

The hard inclusions limit as described in [4] corresponds to the limit $\mathbf{\Gamma} \to \infty$, here we are able to rigorously understand this limit. By what we have established in Proposition 3.2.10, the hard inclusions limit is equivalent to the quadratic minimization Problem 3.2.7.

This limit problem with anisotropic particles prescribing curvatures as in (3.7) is studied in [24]. The elastic interaction energy is calculated and a thermal equilibrium is approximated using a Monte-Carlo algorithm. In the equilibrium configuration proteins aggregate into one region and form an egg carton type structure with the anisotropic particles located at the saddle points of this structure. This equilibrium is analogous to the global minimizer in Problem 3.2.8.

3.3 Numerical experiments

3.3.1 Finite element method

We now consider the numerical approximation of point mean curvature constraints as stated in Problem 3.2.1. We select the solution space

$$\tilde{V} = \{v \in H^4(\Omega) \mid v = 0,\ \Delta v = 0 \text{ on } \partial\Omega\}.$$

Recall this choice of solution space limits us to considering rectangular domains Ω, this will be the case for the remainder of this chapter. Our numerical approximation is based on the penalized formulation of Problem 3.2.3 with $G = (G_i) \in (\tilde{V}')^N$ and $G_i = \delta_{X_i}(\Delta\,\cdot)$ defined in (3.4). We have chosen to study Laplacian constraints as this makes the finite element method much simpler. Recall that the solution to Problem 3.2.3 converges to the solution of Problem 3.2.1 as the penalty parameter ε tends to zero (cf. Remark 3.2.1).

The numerical approximation utilizes a splitting of the eighth order Problem 3.2.3 into an equivalent system of three second order equations for the unknown functions u, $w = \Delta u$ and $z = \Delta w$. For this purpose, we formally rewrite the energy $\tilde{\mathcal{J}}(u)$ defined in (3.5) in terms of w:

$$\frac{1}{2}\int_\Omega \kappa_8(\Delta w)^2 + \kappa_6|\nabla w|^2 + \kappa w^2 + \sigma|\nabla\Delta^{-1}w|^2\,dx + \frac{1}{2\varepsilon}\sum_{k=1}^{N}(\delta_{X_k}w - r_k)^2. \tag{3.28}$$

Note that the corresponding Euler-Lagrange equation is fourth order in w. We impose essential boundary conditions $u = 0$, $w = \Delta u = 0$, and $z = \Delta^2 u = 0$ on $\partial\Omega$.

The rigorous statement of the problem is as follows.

Problem 3.3.1. *Let $p \in (2, \infty)$ and $q \in (1, 2)$ be chosen such that $1/p + 1/q = 1$. Find $(u, w, z) \in H_0^1(\Omega) \times W_0^{1,p}(\Omega) \times W_0^{1,q}(\Omega)$ such that*

$$\begin{aligned} \int_\Omega -\kappa_8 \nabla z \cdot \nabla v + \kappa_6 \nabla w \cdot \nabla v + \kappa w v - \sigma u v \, dx \\ + \frac{1}{\varepsilon} \sum_{k=1}^{N} w(X_k) v(X_k) &= \frac{1}{\varepsilon} \sum_{k=1}^{N} r_k v(X_k), \\ \int_\Omega \nabla u \cdot \nabla v + w v \, dx &= 0, \\ \int_\Omega \nabla w \cdot \nabla v + z v \, dx &= 0 \end{aligned} \tag{3.29}$$

hold for all $v \in W_0^{1,p}(\Omega)$.

Lemma 3.3.1. *The triple (u, w, z) solves Problem 3.3.1 if and only if u solves Problem 3.2.3, $w = \Delta u$ and $z = \Delta w$.*

Proof. The regularity result in Lemma C.2.1 can be applied to u, the solution of Problem 3.3.1. The statement is then proven by arguing as in Lemma 2.4.2. $\square$

The system (3.29) is finally discretised by P^1 finite elements as described in the previous chapter, recall the definition of the usual P^1 finite element space with zero boundary condition

$$V_h := \left\{ v_h \in C^0(\overline{\Omega}) \mid v_h|_K \in P^1(K) \, \forall K \in T_h \text{ and } v_h|_{\partial\Omega} = 0 \right\},$$

we also fix a basis and denote this by

$$\{\phi_1, ..., \phi_{N_h}\}.$$

Note we do not require an approximation to our domain here as in this case Ω is a polygon. The resulting system of equations is:
Find $\mathbf{u}$, $\mathbf{w}$, $\mathbf{z} \in \mathbb{R}^{N_h}$ such that

$$\begin{pmatrix} \kappa_6 S^h + \kappa M^h + \frac{1}{\varepsilon} D^h & -\sigma M^h & -\kappa_8 S^h \\ M^h & S^h & 0 \\ S^h & 0 & M^h \end{pmatrix} \begin{pmatrix} \mathbf{w} \\ \mathbf{u} \\ \mathbf{z} \end{pmatrix} = \begin{pmatrix} \frac{1}{\varepsilon} R^h \\ 0 \\ 0 \end{pmatrix} \tag{3.30}$$

here M^h and S^h are the usual mass and stiffness matrices defined previously. The right hand side vector is given by

$$R_j^h := \sum_{k=1}^{N} r_k \phi_j(X_k).$$

The new matrix, D^h, results from the penalty term and is given by

$$D_{ij}^h := \sum_{k=1}^{N} \phi_i^h(X_k)\phi_j^h(X_k).$$

Notice, due to the localised support of the standard P^1 basis functions, this matrix is sparse, indeed it has the same tridiagonal structure as the mass and stiffness matrices.

We will now present a convergence proof for the above system. We do so by studying a similar but not quite identical system of equations which is equivalent to the one above. First we shall fix some notation.

Definition 3.3.1. *For notational convenience we will label a number of functionals as follows,*

$$\begin{aligned}
c(u,v) &= \int_\Omega \kappa_6 \nabla u \cdot \nabla v + \kappa u v + \frac{1}{\varepsilon}\sum_{i=1}^{N} u(X_i)v(X_i),\\
b_1(u,v) &= \int_\Omega \nabla u \cdot \nabla v,\\
b_2(u,v) &= \kappa_8 \int_\Omega \nabla u \cdot \nabla v,\\
m_1(u,v) &= \int_\Omega uv,\\
m_2(u,v) &= \kappa_8 \int_\Omega uv,\\
F(v) &= -\frac{1}{\varepsilon}\sum_{i=1}^{N} r_i v(X_i).
\end{aligned}$$

Using this notation the finite element problem can now be stated concisely.

Problem 3.3.2. *Find* $(u_h, w_h, z_h) \in V_h \times V_h \times V_h$ *such that*

$$\begin{aligned}
b_2(v_h, z_h) + \sigma m_1(u_h, v_h) + c(w_h, v_h) = F(v_h) \quad \forall v_h \in V_h,\\
b_1(u_h, v_h) - m_1(v_h, w_h) = 0 \quad \forall v_h \in V_h,\\
b_2(w_h, v_h) - m_2(z_h, v_h) = 0 \quad \forall v_h \in V_h.
\end{aligned}$$

Observe that (u_h, w_h, z_h) solves Problem 3.3.2 if and only if

$$u_h = \sum_{i=1}^{N_h} u_i \phi_i, \quad w_h = -\sum_{i=1}^{N_h} w_i \phi_i, \quad z_h = \sum_{i=1}^{N_h} z_i \phi_i,$$

with $(\mathbf{w}, \mathbf{u}, \mathbf{z}) = (w_1, ..., w_{N_h}, u_1, ..., u_{N_h}, z_1, ..., z_{N_h})$ solving (3.30). We will prove convergence for the method. We will require the following inf-sup conditions, they can be proven in a similar manner to Proposition 5.3.1 which appears later in this thesis.

Lemma 3.3.2. *For any $1 < p \leq q < \infty$ such that $1/p + 1/q = 1$ and each $i = 1, 2$ there exist $\beta, \gamma > 0$, independent of h, such that for all $h > 0$*

$$\beta \|\eta_h\|_{1,p} \leq \sup_{v_h \in V_h} \frac{b_i(\eta_h, v_h)}{\|v_h\|_{1,q}} \;\; \forall \eta_h \in V_h \quad \text{and} \quad \gamma \|\xi_h\|_{1,q} \leq \sup_{v_h \in V_h} \frac{b_i(v_h, \xi_h)}{\|v_h\|_{1,p}} \;\; \forall \xi_h \in V_h.$$

Theorem 3.3.1. *For each $h > 0$ there exists a unique $(u_h, w_h, z_h) \in V_h \times V_h \times V_h$ solving Problem 3.3.2. Furthermore*

$$\|u - u_h\|_{1,2} + \|w - w_h\|_{1,2} + \|z - z_h\|_{0,2} \to 0 \text{ as } h \to 0,$$

where u solves Problem 3.2.3, $w = -\Delta u$ and $z = -\Delta w$.

Proof. For existence and uniqueness we need only prove uniqueness of the homogeneous case as the system is linear and finite dimensional. Suppose (u_h, w_h, z_h) solves Problem 3.3.2 with $F = 0$. Then testing the first equation with w_h, the second with σu_h and the third with z_h produces

$$\begin{aligned} b_2(w_h, z_h) + \sigma m_1(u_h, w_h) + c(w_h, w_h) &= 0, \\ \sigma b_1(u_h, u_h) - \sigma m_1(u_h, w_h) &= 0, \\ b_2(w_h, z_h) - m_2(z_h, z_h) &= 0. \end{aligned}$$

Combining the three equations shows

$$m_2(z_h, z_h) + \sigma b_1(u_h, u_h) + c(w_h, w_h) = 0,$$

which implies $z_h = 0$ hence $w_h = 0$ and $u_h = 0$ by using the second and third equations with the inf sup conditions, thus the system is well posed. To show the convergence result we begin by establishing bounds on u_h, w_h and z_h in appropriate norms. First, by the same technique as for the homogeneous system in the proof of uniqueness, it holds

$$\kappa_8 \|z_h\|_{0,2}^2 \leq m_2(z_h, z_h) + \sigma b_1(u_h, u_h) + c(w_h, w_h) = F(w_h).$$

Hence, fixing some $2 < q < \infty$,

$$\|z_h\|_{0,2}^2 \leq C\|F\|\|w_h\|_{1,q}.$$

Now we use the inf sup inequalities in Lemma 3.3.2, by the third equation of the system it follows,

$$\gamma \|w_h\|_{1,q} \leq \sup_{v_h \in V_h} \frac{m_2(z_h, v_h)}{\|v_h\|_{1,p}} \leq C\|z_h\|_{0,2}.$$

Thus, combining the two equations above we obtain

$$\|z_h\|_{0,2} + \|w_h\|_{1,q} \leq C\|F\|.$$

By the second equation of the system it follows

$$\gamma \|u_h\|_{1,q} \leq C\|w_h\|_{0,2}.$$

Finally, fix $1 < p < 2$ such that $1/p + 1/q = 1$ then by the first equation of the system

$$\beta \|z_h\|_{1,p} \leq \frac{1}{\|v_h\|_{1,q}} (F(v_h) - \sigma m_1(u_h, v_h) - c(w_h, v_h)) \leq C(\|F\| + \|u_h\|_{0,2} + \|w_h\|_{1,2}).$$

Thus, combining the above,

$$\|u_h\|_{1,q} + \|w_h\|_{1,q} + \|z_h\|_{1,p} \leq C\|F\|.$$

Hence the sequence (u_h, w_h, z_h) is bounded in $W^{1,q}(\Omega) \times W^{1,q}(\Omega) \times W^{1,p}(\Omega)$ which is a reflexive Banach space. Let h_n be any strictly positive, decreasing sequence such that $h_n \to 0$, thus the sequence $(u^n, w^n, z^n) := (u_{h_n}, w_{h_n}, z_{h_n})$ is a bounded sequence in a reflexive Banach space. Let $(u^{n'}, w^{n'}, z^{n'})$ denote a subsequence which converges weakly, with weak limit (u^*, w^*, z^*). For any $v \in W_0^{1,q}(\Omega)$ there exists a sequence v^n such that $v^n \in V_{h_n}$ for each n and $\|v^n - v\|_{1,q} \to 0$. Thus

$$\begin{aligned} F(v) = \lim_{n' \to \infty} F(v^{n'}) &= \lim_{n' \to \infty} b_2(v^{n'}, z^{n'}) + \sigma m_1(u^{n'}, v^{n'}) + c(w^{n'}, v^{n'}) \\ &= b_2(v, z^*) + \sigma m_1(u^*, v) + c(w^*, v). \end{aligned}$$

Arguing similarly with the two remaining equations produces, for any $v \in H_0^1(\Omega)$,

$$0 = b_1(u^*, v) - m_1(v, w^*),$$
$$0 = b_2(w^*, v) - m_2(z^*, v).$$

Hence $(u^*, w^*, z^*) = (u, -\Delta u, \Delta^2 u)$. As the weakly convergent subsequence was arbitrary it follows $(u^n, w^n, z^n) \rightharpoonup (u, -\Delta u, \Delta^2 u)$ and thus

$$(u_h, w_h, z_h) \rightharpoonup (u, -\Delta u, \Delta^2 u) \text{ in } W^{1,q}(\Omega) \times W^{1,q}(\Omega) \times W^{1,p}(\Omega) \text{ as } h \to 0.$$

By the Sobolev embedding theorem it follows the weak convergence result holds in $H_0^1(\Omega) \times H_0^1(\Omega) \times L^2(\Omega)$ also. Moreover, the embedding $W_0^{1,p}(\Omega) \hookrightarrow L^2(\Omega)$ is compact, hence $\|z_h - \Delta^2 u\|_{0,2} \to 0$, similarly $\|w_h + \Delta u\|_{0,2} \to 0$. Hence

$$b_2(w_h, w_h) = m_2(z_h, w_h) \to m_2(z, -\Delta u) = b_2(-\Delta u, -\Delta u),$$
$$b_1(u_h, u_h) = m_1(u_h, w_h) \to m_1(u, -\Delta u) = b_1(u, u).$$

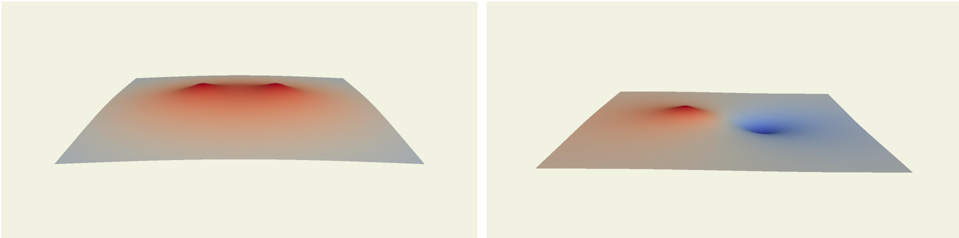
Thus $\|w_h\|_{1,2} \to \|-\Delta u\|_{1,2}$ and $\|u_h\|_{1,2} \to \|u\|_{1,2}$ hence we have strong convergence for u_h and w_h in $H_0^1(\Omega)$.

□

3.3.2 Numerical results

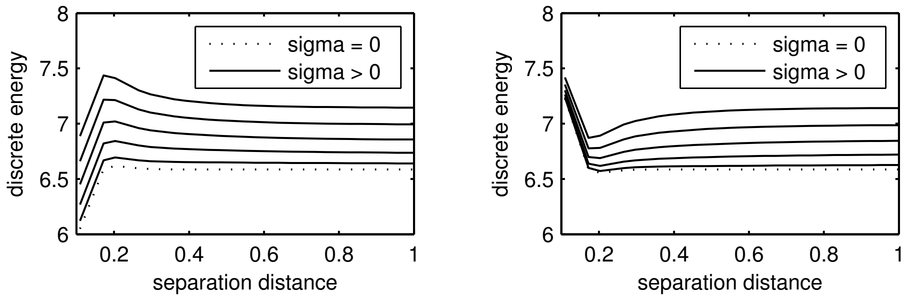
The penalty parameter is taken as $\varepsilon = 1\times 10^{-8}$ in our computations. For the material parameters we use $\kappa_8 = 1.23 \times 10^{-6}$ and $\kappa_6 = 1.11 \times 10^{-3}$, this is justified in the discussion below. We take $\kappa = 1$ and the computational domain to be $\Omega = (-3, 3)^2$ to reduce the effect of the boundary conditions on membrane-mediated interactions.

Figures 3.2a and 3.2b plot the clipping to $(-1, 1)^2$ of the approximate membrane displacement obtained for equal and opposite curvature constraints, respectively, which correspond to equal and opposite orientations of particles. Investigating their interaction potential in analogy to the previous chapter, Figure 3.3a shows that equally oriented particles repel each other for separation distances $R > 0.2$. The strength depends upon membrane tension σ. For distances $R < 0.2$ we observe attraction. For oppositely oriented particles the interaction is repulsive for small and attractive for larger separations as depicted in Figure 3.3b. The strength of the attraction increases with σ.



(a) equally oriented particles (b) oppositely oriented particles

Figure 3.2: Approximate membrane displacement for point mean curvature constraints.



(a) equally oriented particles (b) oppositely oriented particles

Figure 3.3: Interaction potential for point mean curvature constraints over separation distance for $\sigma = 0, 1, 4, 9, 16, 25$ (bottom up).

Discussion

The interaction potential between two particles with circular cross-section has been intensively studied for more than 20 years (see, e.g., [4, 24, 25, 36, 48, 53, 63, 78]), using both point and finite size particles models, here we have focussed on modelling inclusions as points. A comparison of the point inclusion model with the finite sized particle model is made in [31]. This requires a careful consideration of the constants κ_8 and κ_6, along with the specific values for the curvature constraints. The ratios $(\kappa_6/\kappa)^{1/2}$ and $(\kappa_8/\kappa)^{1/4}$ are nanometric lengths and the cutoff length introduced by taking the particles to be points is around $3nm$ (see [4]). By comparing this to the length used in the finite size case, we obtain an appropriate scaling. In the computations described above, we precisely choose the scaling factor $\rho = (\kappa_6/\kappa)^{1/2} = (\kappa_8/\kappa)^{1/4} = 1/30$, this corresponds to both ratios being equal to $1nm$ as the particles have radius around $3nm$ and this is represented by 0.1 in the numerical experiments for finite size particles in [31]. Thus the parameters used are $\kappa = 1$, $\kappa_6 = \rho^2$, $\kappa_8 = \rho^4$ and $r_k = \pm 20$, the latter is obtained for circular particles of radius 0.1 via equation (3.3). Thus, separation distances shorter than $R = 0.2$ are physically impossible, as they represent situations where particles overlap. This explains and contextualises the observed unphysical interactions for short distances $R < 0.2$. For comparison with the results obtained for the finite-sized circular particles, it is therefore sufficient to consider separation distances $R \geq 0.2$. The major difference is that the point model does not reproduce the strong repulsion at the limiting separation $R = 0.2$. This is unsurprising as the point model introduces a cutoff length similar to the length the strong repulsion acts over. For separation distances above this cutoff i.e., for $R > 0.3$, the observed interactions agree qualitatively and quantitatively with the finite size case.

For finite-size particles Weikl, Kozlov & Helfrich [78] found by analytical considerations that in case of positive membrane tension, i.e., $\sigma > 0$, the interaction depends on the relative orientation of the two particles: Equally oriented particles repel each other at all separation distances, whereas for particles with opposite orientation the interaction is repulsive at small and attractive at larger distances. For $\sigma = 0$ the interaction is found to be repulsive at all distances independent of the particles' orientation, confirming earlier results for finite-size particles in [36, 48, 63]. Similar results have been obtained for point-like particles [4, 24, 53]. These theoretical findings are in accordance with our numerical computations. Note that well-known interaction laws of the form $1/R^4$ for circular particles are based on large distance asymptotics assuming an unbounded asymptotically flat membrane with particles separated by distances which are large compared to their size, i.e. $r \ll R$. Our numerical experiments, however, cover the complementary situation $r \approx R$.

Chapter 4

Small deformations of Willmore surfaces

4.1 Notation and preliminaries

We now move on to formulating membrane models based on deformations of a more general surface. To do so we must fix some notation related to the geometrical concepts involved, principally the notion of a surface derivative. Much of the following material is taken from [27] which provides a more detailed explanation of the required concepts.

In the following we consider an embedding $x : \mathcal{M} \to \mathbb{R}^3$ of a two-dimensional connected, closed (that is compact and without boundary), orientable manifold (that is a topological space which is locally homeomorphic to open subsets Ω_i of $\mathbb{R}^2$ via the so-called coordinate charts $\mathcal{C}_i : U_i \subset \mathcal{M} \to \Omega_i \subset \mathbb{R}^2$). In the following we assume that $\mathcal{M}$ and x are as regular as needed, but at most of class C^4. The image $\Gamma := x(\mathcal{M})$ of $\mathcal{M}$ is a two-dimensional connected, closed, orientable hypersurface embedded into $\mathbb{R}^3$.

Henceforward, the Euclidean scalar product is denoted by $v \cdot w := v_\alpha w_\alpha$, where we have made use of the convention to sum over repeated indices. For matrices $A, B \in \mathbb{R}^{3\times 3}$ we define the scalar product $A : B := A_{\alpha\beta} B_{\alpha\beta}$.

According to the Jordan-Brouwer separation theorem, see [52], there exists a bounded domain D which has Γ as its point set boundary. The unit normal ν to Γ that points away from this domain is called the outward unit normal. We define $P := \mathbb{1} - \nu \otimes \nu$ on Γ to be, at each point of Γ, the projection onto the corresponding tangent space. Here $\mathbb{1}$ denotes the identity matrix in $\mathbb{R}^3$. For a differentiable function f on Γ we define the tangential gradient by

$$\nabla_\Gamma f := P\nabla\overline{f},$$

where $\overline{f}$ is a differentiable extension of f to an open neighbourhood of $\Gamma \subset \mathbb{R}^3$. Here, ∇ denotes the usual gradient in $\mathbb{R}^3$. The above definition only depends on the values of f on Γ. In particular, it does not depend on the extension $\overline{f}$, see Lemma 2.4 in [27] for more details. The components of the tangential gradient are denoted by $(\underline{D}_1 f, \underline{D}_2 f, \underline{D}_3 f)^T := \nabla_\Gamma f$. For a twice differentiable function the Laplace-Beltrami operator is defined by

$$\Delta_\Gamma f := \nabla_\Gamma \cdot \nabla_\Gamma f.$$

The extended Weingarten map $\mathcal{H} := \nabla_\Gamma \nu$ is symmetric and has zero eigenvalue in the normal direction. The eigenvalues κ_i, $i = 1, 2$, belonging to the tangential eigenvectors are the principal curvatures of Γ. The mean curvature H is the sum of the principal curvatures, that is $H := \sum_{i=1}^2 \kappa_i = \text{trace}\,(\mathcal{H}) = \nabla_\Gamma \cdot \nu$. Note that our definition differs from the more common one by a factor of 2. We will denote the identity function on Γ by id_Γ, that is $id_\Gamma(p) = p$ for all $p \in \Gamma$. The mean curvature vector $H\nu$ satisfies $H\nu = -\Delta_\Gamma id_\Gamma$, see Section 2.3 in [18]. Tangential gradients satisfy the following commutator rule, see Lemma 2.6 in [27],

$$\underline{D}_\alpha \underline{D}_\beta f - \underline{D}_\beta \underline{D}_\alpha f = \left(\mathcal{H}\nabla_\Gamma f\right)_\beta \nu_\alpha - \left(\mathcal{H}\nabla_\Gamma f\right)_\alpha \nu_\beta. \tag{4.1}$$

The Sobolev spaces $H^1(\Gamma)$ and $H^2(\Gamma)$ on the hypersurface Γ are defined by

$$H^1(\Gamma) := \left\{ f \in L^2(\Gamma) \mid f \text{ has weak derivatives } \underline{D}_\alpha f \in L^2(\Gamma),\ \alpha = 1,2,3 \right\},$$
$$H^2(\Gamma) := \left\{ f \in H^1(\Gamma) \mid \text{all weak derivatives } \underline{D}_\beta \underline{D}_\alpha f \in L^2(\Gamma),\ \alpha,\beta = 1,2,3 \text{ exist} \right\},$$

where $\underline{D}_\alpha f := v_\alpha \in L^2(\Gamma)$ is said to be the weak derivative of f if

$$\int_\Gamma f \underline{D}_\alpha \phi \, do = -\int_\Gamma v_\alpha \phi \, do + \int_\Gamma f\phi H \nu_\alpha \, do$$

for all smooth test functions ϕ on Γ, see also Definition 2.11 in [27]. Here, the integrals are taken with respect to the two-dimensional Hausdorff measure on Γ. The Sobolev space $H^1(\Gamma)$ is a Hilbert space when endowed with the standard H^1 inner product and induced norm,

$$(u,v)_{H^1(\Gamma)} := \int_\Gamma \nabla_\Gamma u \cdot \nabla_\Gamma v + uv \, do \quad \text{and} \quad \|u\|_{H^1(\Gamma)} := \sqrt{(u,u)_{H^1(\Gamma)}}.$$

Similarly, $H^2(\Gamma)$ is a Hilbert space when endowed with the following inner product and induced norm

$$(u,v)_{H^2(\Gamma)} := \int_\Gamma \Delta_\Gamma u \Delta_\Gamma v + \nabla_\Gamma u \cdot \nabla_\Gamma v + uv \; do \quad \text{and} \quad \|u\|_{H^2(\Gamma)} := \sqrt{(u,u)_{H^2(\Gamma)}}.$$

Observe we are not using the standard inner product and induced norm on $H^2(\Gamma)$ which contains mixed second order derivatives. On a closed surface however the norm we defined above is equivalent to the standard $H^2(\Gamma)$ norm, see [27, Lemma 3.2] for details.

We next assume that $\Gamma_s := x_s(\mathcal{M})$ depends on a parameter $s \in (-\delta, \delta)$, $\delta > 0$. The material derivative $\dot{f}$ of a function $f : \bigcup_{s\in(-\delta,\delta)} \Gamma_s \times \{s\} \to \mathbb{R}$ is then defined by

$$\dot{f} := \frac{\partial (f \circ x_s)}{\partial s} \circ x_s^{-1}. \tag{4.2}$$

We will also use the notation $\dot{\partial} f$ to denote the material derivative. The transport formula, see Theorem 5.1 in [27], states that

$$\frac{d}{ds} \int_{\Gamma_s} f \; do_s = \int_{\Gamma_s} \dot{f} + f \; \nabla_{\Gamma_s} \cdot V \; do_s, \tag{4.3}$$

where the vector field V on Γ_s is given by $V \circ x_s := \frac{\partial}{\partial s} x_s$. If $X(\theta)$ is a local parametrization of Γ, see [27, Section 2] , the first fundamental form $G(\theta) := (g_{ij}(\theta))_{i,j=1,2}$ has entries

$$g_{ij}(\theta) := \frac{\partial X}{\partial \theta_i} \cdot \frac{\partial X}{\partial \theta_j}.$$

The matrix G is invertible and we denote the entries of G^{-1} by g^{ij}.

4.2 Modelling of small surface deformations without surface tension

4.2.1 Deformations due to small external forces

We begin by considering surfaces without tension, that is we model their energy by the functional $\mathcal{J}_{CH}$ in (2.1). As previously, we will consider zero spontaneous curvature and may negate the Gaussian curvature term as we will work with closed surfaces, so this term is simply a constant. In this case we fix the constant $\kappa = 1$ since its only effect is to rescale the energy. The resulting energy functional is the

Willmore functional and here we denote it by W, that is

$$W(\Gamma) := \int_\Gamma \frac{1}{2} H^2 \, do. \tag{4.4}$$

In the following we will consider surfaces which are critical points for the energy W, we will denote these by Γ_0. This means that Γ_0 satisfies

$$\frac{d}{ds} W(\Gamma_s)\bigg|_{s=0} = 0, \qquad \forall u \in C^2(\Gamma_0). \tag{4.5}$$

where $\Gamma_s := \{p + su(p)\nu(p) \mid p \in \Gamma_0\}$. We will refer to Γ_0 as an undeformed surface. We now discuss how small deformations that are due to some small external forces can be incorporated into this model by perturbing the energy functional.

The undeformed membrane Γ_0 is now exposed to some external forces. Since the exact form of the forces is negligible in this section, we describe them by some arbitrary (non-linear) energy functional $\tilde{\mathcal{F}}(\Gamma)$. In Section 4.4 we will discuss point forces in detail. Such forces can indeed be regarded as a model for forces acting on biomembranes in living cells. We say that a force is small if the associated energy functional is small compared to the change in the bending energy. In this case we rescale the functional $\tilde{\mathcal{F}}$ by a small parameter $\varepsilon > 0$, that is $\mathcal{F} := \tilde{\mathcal{F}}/\varepsilon$, such that the rescaled energy $\mathcal{F}$ is of the same order as the change in the bending energy. For such forces the total energy of the membrane is given by

$$\mathcal{J}_\varepsilon(\Gamma) := W(\Gamma) - \varepsilon \mathcal{F}(\Gamma). \tag{4.6}$$

We are motivated by attempting to minimise this energy. Since the energy associated to the external forces is of order ε we regard this as a perturbation of the Willmore energy W. It is then reasonable to assume that the deformation is also of order ε and that a deformed surface Γ can be described as a graph over Γ_0, explicitly deformed surfaces are of the form

$$\Gamma_\varepsilon := \{p + \varepsilon(u\nu)(p) \mid p \in \Gamma_0\}, \tag{4.7}$$

where the height function $u \in C^2(\Gamma_0)$ is defined on the undeformed membrane Γ_0. It describes the deformations of Γ_0 in the normal direction that are induced by the external forces. We wish to find the deformed surface Γ_ε for which the energy (4.6) is least. In the following we aim to find a good approximation for the above energy which will simplify energy minimisation to a linear PDE. We first note that the energy $\mathcal{J}_\varepsilon$ can be interpreted as a functional for the height function u which depends on a scale parameter ε. With a slight abuse of notation, we therefore write $\mathcal{J}_\varepsilon(u)$ instead of $\mathcal{J}_\varepsilon(\Gamma_\varepsilon)$ in the following. We now treat $\mathcal{J}_\varepsilon(u)$ as a function of a single variable ε and produce the following second order Taylor expansion

$$\mathcal{J}_\varepsilon(u) = \mathcal{J}_0(u) + \varepsilon \frac{\mathrm{d}\mathcal{J}_\varepsilon(u)}{\mathrm{d}\varepsilon}\bigg|_{\varepsilon=0} + \frac{\varepsilon^2}{2}\frac{\mathrm{d}^2\mathcal{J}_\varepsilon(u)}{\mathrm{d}\varepsilon^2}\bigg|_{\varepsilon=0} + O(\varepsilon^3). \tag{4.8}$$

We observe that the first term $\mathcal{J}_0(u) = W(\Gamma_0)$ does not depend on u. Since Γ_0 is assumed to be a critical point of W, the second term reduces to $-\mathcal{F}(\Gamma_0)$ and thus does not depend on u. The second order term is therefore the lowest order term that depends on u. The Taylor expansion hence can be written as

$$\mathcal{J}_\varepsilon(u) = W(\Gamma_0) - \varepsilon\mathcal{F}(\Gamma_0) + \varepsilon^2 J(u) + O(\varepsilon^3).$$

with

$$J(u) := \frac{1}{2}\frac{\mathrm{d}^2\mathcal{J}_\varepsilon(u)}{\mathrm{d}\varepsilon^2}\bigg|_{\varepsilon=0}. \tag{4.9}$$

The approximate energy $J(u)$ is the sum of variations of the functionals W and $\mathcal{F}$. To derive an explicit formula for $J(u)$ will be part of the next section. Instead of determining minimisers of the original energy in (4.6), we aim to approximate them by considering the novel energy J.

4.2.2 Derivation of an energy functional for the height function

In this section we discuss the first and second variations of $W(\Gamma)$. We first consider variations $\Gamma_\varepsilon := \{p + \varepsilon(u\nu)(p) \mid p \in \Gamma\}$ on arbitrary surfaces Γ before we restrict the results to Γ_0. We will then use these results in (4.9) to obtain an explicit formula for $J(u)$. In the next sections we will discuss the application of this result to the deformation of spheres and Clifford tori.

First and second variations

In the following we will usually state the results of the first and second variations without using integration by parts and we will note it explicitly if a formula is based on integration by parts. Whilst this distinction is minor in the present work, there are several reasons why it is quite useful to separate these results from each other:

1. Using integration by parts requires higher regularity of the surface Γ or of the embedding x, respectively.

2. The approach presented here could be extended to surfaces with boundary, in which case boundary conditions have to be taken into account. To consider surfaces with boundary might indeed be interesting in order to model finite size inclusions in biomembranes.

3. On piecewise linear interpolations of the surface Γ, see Section 4.6, integration by parts would lead to additional terms depending on the discontinuous co-normals of the mesh simplices. This means that the discretisation of formulas, which are equivalent in the smooth case, usually leads to different algorithms. Therefore, one has to be very careful in numerics, which formula one chooses for the discretisation.

To compute the required derivatives of W we use the following formulae relating them to variations of W,

$$\begin{aligned} W'(\Gamma)[u\nu] &:= \left.\frac{\mathrm{d}W(\Gamma_\varepsilon)}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0}, \\ W''(\Gamma)[u\nu, u\nu] &:= \left.\frac{\mathrm{d}^2W(\Gamma_\varepsilon)}{\mathrm{d}\varepsilon^2}\right|_{\varepsilon=0}. \end{aligned}$$

Remark 4.2.1. *In the following we assume sufficient smoothness of u and Γ, however we require at most C^4 regularity. The functionals, which we will obtain below from the second variation, can then be extended to $u \in H^2(\Gamma)$ using density arguments.*

Remark 4.2.2. *By definition the first and second variation of a functional F at the point p in the direction of v is*

$$F'(p)[v] := \left.\frac{d\phi(\varepsilon)}{d\varepsilon}\right|_{\varepsilon=0}, \quad \text{and} \quad F''(p)[v,v] := \left.\frac{d^2\phi(\varepsilon)}{d\varepsilon^2}\right|_{\varepsilon=0},$$

where $\phi(\varepsilon) := F(p + \varepsilon v)$, see, for example, page 688 ff. in [85]. However, note that the second variations presented below and in the Appendix are based on the variation of the first variation, that is on

$$\left.\frac{d\varphi(\mu)}{d\mu}\right|_{\mu=0} \quad \text{with} \quad \varphi(\mu) := (F'[v])(p + \mu v).$$

So, the question is whether this gives the correct expression for the second variation of the considered functionals. In general this is not quite clear since $\varphi(\mu) \neq \frac{d\phi}{d\varepsilon}\big|_{\varepsilon=\mu}$. This condition will hold for each of our applications however. For example, for the *functional $F = W$, we have*

$$\varphi(\mu) = W'(\Gamma_\mu)[u^\ell \nu^\mu], \quad \text{whereas} \quad \left.\frac{d\phi}{d\varepsilon}\right|_{\varepsilon=\mu} = W'(\Gamma_\mu)[u^\ell \nu^\ell].$$

Here, $\Gamma_\mu := \{c_\mu(p) \mid p \in \Gamma\}$ is the deformed surface with outward unit normal ν^μ, where c_μ is defined by $c_\mu := id_\Gamma + \mu u \nu$, and $u^\ell := u \circ c_\mu^{-1}$ is the lift of u onto Γ_μ. Note that $\nu^\ell := \nu \circ c_\mu^{-1}$ is the lift of the outward unit normal ν to Γ onto Γ_μ. Using the embedding $x : \mathcal{M} \to \Gamma$ for Γ, an embedding x_μ for Γ_μ is given by $x_\mu := c_\mu \circ x$. The material derivative (4.2) with respect to x_μ of u^ℓ and ν^ℓ is, in fact, zero. On the other hand, the material derivative of ν^μ usually does not vanish. We therefore find that

$$\left.\frac{d^2\phi(\varepsilon)}{d\varepsilon^2}\right|_{\varepsilon=0} - \left.\frac{d\varphi(\mu)}{d\mu}\right|_{\mu=0} = -W'(\Gamma)[u\dot{\partial}\nu].$$

Since the material derivative $\dot{\partial}\nu$ is a tangent vector field to Γ, it follows from the invariance of $W(\Gamma)$ under diffeomorphisms, that the first variation of $W(\Gamma)$ in the direction of $\dot{\partial}\nu$ vanishes. We hence obtain that

$$\left.\frac{d^2\phi(\varepsilon)}{d\varepsilon^2}\right|_{\varepsilon=0} = \left.\frac{d\varphi(\mu)}{d\mu}\right|_{\mu=0}.$$

The same applies to the other functionals considered in this text.

The following results hold on arbitrary (sufficiently smooth) surfaces Γ (with or without boundary).

$$W'(\Gamma)[u\nu] = \int_\Gamma -H\left(\Delta_\Gamma u + |\mathcal{H}|^2 u - \frac{1}{2}H^2 u\right)\, do, \tag{4.10}$$

$$\begin{aligned} W''(\Gamma)[u\nu, g\nu] = \int_\Gamma &(\Delta_\Gamma g + |\mathcal{H}|^2 g)(\Delta_\Gamma u + |\mathcal{H}|^2 u) + 2H\mathcal{H} : (g\nabla_\Gamma\nabla_\Gamma u + u\nabla_\Gamma\nabla_\Gamma g) \\ &+ 2H\mathcal{H}\nabla_\Gamma u \cdot \nabla_\Gamma g + Hg\nabla_\Gamma u \cdot \nabla_\Gamma H - H^2\nabla_\Gamma u \cdot \nabla_\Gamma g - \frac{3}{2}H^2 u\Delta_\Gamma g - H^2 g\Delta_\Gamma u \\ &+ \left(2HTr(\mathcal{H}^3) - \frac{5}{2}H^2|\mathcal{H}|^2 + \frac{1}{2}H^4\right) gu\, do. \end{aligned} \tag{4.11}$$

This follows from (D.1) and Theorem D.1.1 in the appendix. In order to derive the above formula we have not used integration by parts. It might therefore also be applied to surfaces with boundary. Here we restrict to closed surfaces. Integration by parts then gives, see also Remark D.1.1,

$$
\begin{aligned}
W''(\Gamma)[u\nu, g\nu] = \int_\Gamma & (\Delta_\Gamma g + |\mathcal{H}|^2 g)(\Delta_\Gamma u + |\mathcal{H}|^2 u) + 2H\mathcal{H} : (g\nabla_\Gamma\nabla_\Gamma u + u\nabla_\Gamma\nabla_\Gamma g) \\
& + 2H\mathcal{H}\nabla_\Gamma u \cdot \nabla_\Gamma g - \frac{3}{2}H^2\nabla_\Gamma u \cdot \nabla_\Gamma g - \frac{3}{2}H^2(u\Delta_\Gamma g + g\Delta_\Gamma u) \\
& + \left(2HTr(\mathcal{H}^3) - \frac{5}{2}H^2|\mathcal{H}|^2 + \frac{1}{2}H^4\right) gu \, do.
\end{aligned}
\tag{4.12}
$$

The first variation of the Willmore energy can be found in [81]. The formula for the second variation was obtained in [35]. For the sake of completeness, we also present its derivation in the appendix, since it is indeed a crucial part of this work. Recall that we assume Γ_0 is chosen so that the first variation term vanishes, see (4.5).

To complete the calculation of $J(u)$, defined in (4.9), we require the second derivative of the force term,

$$
\left.\frac{\mathrm{d}^2(\varepsilon\mathcal{F}(\Gamma_\varepsilon))}{\mathrm{d}\varepsilon^2}\right|_{\varepsilon=0} = 2\mathcal{F}'(\Gamma_0)[u\nu].
$$

Here we have applied the definition of the first variation given in Remark 4.2.2. The functional J is a novel quadratic energy with which we will formulate the variational problems related to the surface displacement.

Definition 4.2.1. *Given a surface $\Gamma_0 \subset \mathbb{R}^3$, we define the quadratic surface energy $J : H^2(\Gamma_0) \to \mathbb{R}$ by*

$$
J(u) := \frac{1}{2}\left.\frac{\mathrm{d}^2\mathcal{J}_\varepsilon(u)}{\mathrm{d}\varepsilon^2}\right|_{\varepsilon=0} = \frac{1}{2}W''(\Gamma_0)[u\nu, u\nu] - \mathcal{F}'(\Gamma_0)[u].
$$

Under the assumption Γ_0 is chosen such that the first variation $W'(\Gamma_0)$ vanishes, by the Taylor expansion (4.8), $J(u)$ is an $O(\varepsilon^3)$ order approximation of $\mathcal{J}_\varepsilon(u)$, up to an additive constant.

Lemma 4.2.1. *For an undeformed surface $\Gamma_0 \subset \mathbb{R}^3$ chosen such that $W'(\Gamma_0)$ vanishes we have*

$$
\mathcal{J}_\varepsilon(u) = W(\Gamma_0) - \varepsilon\mathcal{F}(\Gamma_0) + \varepsilon^2 J(u) + O(\varepsilon^3).
$$

Henceforward, we will neglect the constant and the $O(\varepsilon^3)$ terms. We interpret J as a new energy. We aim to minimize this energy in the next sections. This is of course only possible if the total energy is bounded from below. Since we want to determine minimizers by considering the associated variational problems, and in particular compute numerical approximations, we limit the space of admissible variations so that the bilinear form corresponding to the second variation term $W''(\Gamma_0)[\cdot\nu, \cdot\nu]$ is coercive in the $H^2(\Gamma_0)$-norm over this space. Note that in [75], it was recently proved that Willmore immersions are local minimizers if the second variation of the Willmore functional is positive semi-definite with kernel equal to the sum of the space of infinitesimal Möbius transformations and of the space of tangential variations. In this chapter we shall consider the case that Γ_0 is a sphere or a Clifford torus and the latter condition is satisfied. Furthermore we only consider normal variations, thus there is a space of admissible variations with finite codimension over which we are able to formulate well-posed problems.

4.2.3 Application to the Monge gauge

Before proceeding to curved surfaces we will first examine the quadratic surface energy in Definition 4.9 in the Monge gauge used in Chapter 2. In this setting the undeformed surface is chosen to be a planar domain, that is $\Gamma_0 = \Omega \times \{0\}$ for some bounded domain $\Omega \subset \mathbb{R}^2$. The normal to the surface is given by $\nu = (0, 0, 1)$ and does not vary over the surface, hence $H = 0$ and the Weingarten map $\mathcal{H}$ is the zero matrix. By (4.10) it follows $W'(\Gamma_0)$ vanishes and we may apply the linearisation derived above. Inserting this choice for Γ_0 into (4.11) produces

$$W''(\Gamma_0)[u\nu, g\nu] = \int_{\Gamma_0} \Delta_{\Gamma_0} u \Delta_{\Gamma_0} g \, do.$$

Parametrising Ω by two dimensional Cartesian coordinates (x_1, x_2), observe in this case the tangential gradient is given by

$$\nabla_{\Gamma_0} u(x_1, x_2, 0) = (\partial_{x_1} u(x_1, x_2, 0), \partial_{x_2} u(x_1, x_2, 0), 0)$$

for any sufficiently smooth function $u : \Gamma_0 \to \mathbb{R}$. It follows that the Laplace-Beltrami operator is simply the two dimensional Laplacian,

$$\Delta_{\Gamma_0} u = \partial_{x_1 x_1} u + \partial_{x_2 x_2} u.$$

The second variation of the Willmore functional thus produces the term proportional to κ in the classical Monge gauge linearisation (2.7). The σ term arises from the treatment of surface tension, this may be done analogously to the sphere which appears later in this chapter.

4.2.4 The kernel of $W''(\Gamma_0)$ in the cases of a sphere and a Clifford torus

We now examine the undeformed surfaces $\Gamma_0 = S(0, R)$, a sphere with radius R centred at the origin and $\Gamma_0 = T(R, R\sqrt{2})$, a Clifford torus with tube radius R centred at the origin. Both of these surfaces are Willmore surfaces, that is $W'(\Gamma_0)$ vanishes. The quadratic surface energy is given by

$$J(u) = \frac{1}{2}a(u, u) - \mathcal{F}'(\Gamma_0)[u],$$

where we have introduced the bilinear form $a : H^2(\Gamma_0) \times H^2(\Gamma_0) \to \mathbb{R}$ defined by

$$a(u, v) := W''(\Gamma_0)[u\nu, v\nu]. \tag{4.13}$$

The bilinear form is bounded, symmetric and positive semi-definite, for the sphere this is immediate from Corollary D.1.2 in the appendix, for the Clifford torus see [58, 79]. As remarked above, to formulate well-posed problems we will work in a subspace of $H^2(\Gamma_0)$ over which $a(\cdot, \cdot)$ is coercive. To find such a subspace one must first identify the kernel of a, that is the set

$$Ker(a) := \left\{ v \in H^2(\Gamma_0) \mid a(v, w) = 0 \ \forall w \in H^2(\Gamma_0) \right\}.$$

For both the sphere and Clifford torus the kernel is finite dimensional, we will identify a basis in each case, that is we will write the kernel in the form

$$Ker(a) = sp \left\{ f_1, ..., f_M \right\},$$

for some $M := dim(Ker(a)) \geq 1$. This is done in the following lemma.

Lemma 4.2.2. *Let $\nu_1, \nu_2, \nu_3 : \Gamma_0 \to \mathbb{R}$ denote the components of the outward normal vector field ν_{Γ_0}.*

- *If Γ_0 is a sphere or a Clifford torus then*

$$\begin{aligned} Ker(a) &= Moeb(\mathbb{R}^3) \cdot \nu_{\Gamma_0} \\ &:= \left\{ u \in H^2(\Gamma_0) \mid u(x) = f(x) \cdot \nu_{\Gamma_0}(x) \text{ for some } f \in Moeb(\mathbb{R}^3) \right\}. \end{aligned}$$

- *If Γ_0 is a sphere then*

$$Ker(a) = sp \left\{ 1, \nu_1, \nu_2, \nu_3 \right\}.$$

- *If Γ_0 is a Clifford torus then*

$$
\begin{aligned}
Ker(a) = sp\,\{\nu_1, \nu_2, \nu_3, f_4(x) &:= x_3\nu_1 - x_1\nu_3, f_5(x) := x_3\nu_2 - x_2\nu_3, \\
& f_6(x) := x \cdot \nu, f_7(x) := 2x_1(x \cdot \nu) - |x|^2\nu_1, \\
& f_8(x) := 2x_2(x \cdot \nu) - |x|^2\nu_2\}\,.
\end{aligned}
$$

- *If Γ_0 is a sphere or Clifford torus then there exists $C(\Gamma_0) > 0$ such that*

$$a(v,v) \geq C(\Gamma_0)\|v\|_{H^2(\Gamma_0)} \quad \forall v \in Ker(a)^\perp,$$

where $\perp$ denotes orthogonality with respect to the $H^2(\Gamma_0)$ inner product.

Here $Moeb(\mathbb{R}^3)$ denotes the set of infinitesimal Möbius transformations on $\mathbb{R}^3$. For an abstract definition of this set see [66], here we will use an equivalent characterisation, also presented in [66].

Proof. We begin with $\Gamma_0 = S(0,R)$, a sphere. The bilinear form a is explicitly calculated in the appendix as Corollary D.1.2. Here we consider $n = 2$, hence the bilinear form is given by

$$a(u,v) = \int_{\Gamma_0} \Delta_{\Gamma_0} u \Delta_{\Gamma_0} v - \frac{2}{R^2} \nabla_{\Gamma_0} u \cdot \nabla_{\Gamma_0} v \; do$$

Note that $1 \in Ker(a)$ and that, on a sphere, each component of the normal ν_i is an eigenfunction of $-\Delta_{\Gamma_0}$ with eigenvalue $2/R^2$, hence

$$Sp\,\{1, \nu_1, \nu_2, \nu_3\} \subset Ker(a). \tag{4.14}$$

To obtain equality in this inclusion and prove the coercivity statement for a sphere we will use the following Poincaré inequality.

$$\int_{\Gamma_0} u^2 \; do \leq \frac{R^2}{6} \int_{\Gamma_0} |\nabla_{\Gamma_0} u|^2 \; do \leq \frac{R^4}{36} \int_{\Gamma_0} (\Delta_{\Gamma_0} u)^2 \; do \quad \forall u \in Sp\,\{1, \nu_1, \nu_2, \nu_3\}^\perp\,, \tag{4.15}$$

where again $\perp$ denotes orthogonality with respect to the $H^2(\Gamma_0)$ inner product. To prove this, note for a sphere of radius R the negative Laplace-Beltrami operator, $-\Delta_\Gamma$, has eigenvalues

$$\lambda_k = \frac{k(k+1)}{R^2} \quad \text{with multiplicities} \quad N_k = \binom{k+2}{2}, \quad k \in \mathbb{N} \cup \{0\}\,.$$

See [74] for a proof on the unit sphere, from which we deduce the above. It follows that $\lambda_0 = 0$ and $N_0 = 1$, thus the zero eigenfunctions are simply constant functions. The next eigenvalue $\lambda_1 = 2/R^2$ has multiplicity $N_1 = 3$. We then see the λ_1-eigenfunctions are spanned by $\{\nu_1, \nu_2, \nu_3\}$. Thus the optimal Poincaré constant over $Sp\{1, \nu_1, \nu_2, \nu_3\}^\perp$, C_P, satisfies

$$C_P^{-2} = \inf_{v \in S} \frac{\int_\Gamma |\nabla_\Gamma v|^2 \, do}{\int_\Gamma v^2 \, do} = \lambda_2$$

where $S := \left\{u \in H^1(\Gamma_0) \mid 0 = \int_\Gamma u \, do = \int_\Gamma u\nu_i \, do, \; i = 1, 2, 3\right\}$ and λ_2 is the second non-zero eigenvalue for the negative Laplace-Beltrami operator. The validity of the inequality used above relies upon the fact that $H^2(\Gamma_0) \cap S = Sp\{1, \nu_1, \nu_2, \nu_3\}^\perp$, that is for $H^2(\Gamma_0)$ functions, membership of S encodes both L^2 and H^2 orthogonality to $Ker(a)$. To see this, a simple calculation shows

$$\begin{aligned} (u, 1)_{H^2(\Gamma_0)} &= (u, 1)_{L^2(\Gamma_0)} && \forall u \in H^2(\Gamma_0), \\ (u, \nu_i)_{H^2(\Gamma_0)} &= \left(\tfrac{4}{R^4} + \tfrac{2}{R^2} + 1\right)(u, \nu_i)_{L^2(\Gamma_0)} && \forall u \in H^2(\Gamma_0). \end{aligned} \tag{4.16}$$

For a sphere $\lambda_2 = 6/R^2$, proving the first inequality in (4.15). The second inequality then follows by integration by parts and the Hölder inequality. Coercivity of $a(\cdot, \cdot)$ over $Sp\{1, \nu_1, \nu_2, \nu_3\}^\perp$ follows from (4.15). From this we deduce equality in (4.14) and coercivity of $a(\cdot, \cdot)$ over $Ker(a)^\perp$ for a sphere.

For Γ_0 a Clifford torus the first and final statements in this lemma are proven in [58, 75]. For the remaining two statements we use the characterisation of $Moeb(\mathbb{R}^3)$ given in [66],

$$f \in Moeb(\mathbb{R}^3) \text{ if and only if } f(x) = a + (K + \alpha \mathbb{1})x + 2(b \cdot x)x - |x|^2 b$$

where $\alpha \in \mathbb{R}$, $a, b \in \mathbb{R}^3$, $\mathbb{1} \in \mathbb{R}^{3\times 3}$ is the identity matrix and $K \in \mathbb{R}^{3\times 3}$ is a skew-symmetric matrix. We may regard $Moeb(\mathbb{R}^3)$ as a 10 dimensional subspace of $C^\infty(\mathbb{R}^3)$ and can thus determine $Moeb(\mathbb{R}^3) \cdot \nu_{\Gamma_0}$ for each of our choices of Γ_0, using a suitable parametrisation of each surface. $\square$

Note that the kernel is not 10 dimensional in either case. This is due to the fact that for some infinitesimal Möbius transformations f, $f(x)$ lies in the tangent plane to Γ_0 for each $x \in \Gamma_0$. Working over $Ker(a)^\perp$ we are able to formulate well posed mathematical problems. One can justify this step physically as non admissible variations are those which alter the surface but do not change the Willmore energy W up to second order.

As we will work with $Ker(a)^\perp$ frequently it is useful to detail three methods by which this set can be characterised. Firstly, the standard definition gives

$$Ker(a)^\perp = \left\{v \in H^2(\Gamma_0) \mid (v,w)_{H^2(\Gamma_0)} = 0 \;\forall w \in Ker(a)\right\}.$$

Secondly, by writing $Ker(a) = sp\{f_1, ..., f_M\}$, it follows

$$Ker(a)^\perp = \left\{v \in H^2(\Gamma_0) \mid (v,f_i)_{H^2(\Gamma_0)} = 0 \;\forall 1 \le i \le M\right\}.$$

Finally, it follows from our choice of $H^2(\Gamma_0)$ inner product that

$$Ker(a)^\perp = \left\{v \in H^2(\Gamma_0) \mid (v,g_i)_{L^2(\Gamma_0)} = 0 \;\forall 1 \le i \le M\right\},$$

where $g_i := (\Delta_{\Gamma_0}^2 - \Delta_{\Gamma_0} + 1)f_i$. This characterisation follows by integrating the $H^2(\Gamma_0)$ inner product by parts, notice each f_i is sufficiently regular to permit this.

4.3 A spherical membrane under tension

We now consider a spherical membrane, $\Gamma_0 = S(0, R)$, with positive surface tension $\sigma > 0$, with the surface energy functional $\mathcal{J}_{CH}$ given in (2.2), again we consider zero spontaneous curvature and negate the Gaussian curvature term. Note that we will only consider spherical membranes when considering a positive surface tension. To formulate relevant minimisation problems we also introduce a fixed volume constraint. This is required as W, the Willmore energy, is scale invariant but the surface tension term proportional to σ is not.

The fixed volume constraint is physically reasonable. Biological membranes are usually semipermeable, which means that certain molecules or ions cannot diffuse through the membrane, whereas this is possible for other molecules like water. If such a membrane is contained in an isotonic environment, that is a solvent which has the same effective solute concentration as the solution enclosed by the membrane, the volume enclosed by this membrane does not change.

We therefore here assume that the volume enclosed by our deformed hypersurface Γ is a constant given by $V_0 > 0$. Let $D \subset \mathbb{R}^3$ denote the bounded domain which has Γ as its point boundary set. Then the volume of D is given by

$$|D| := \int_D 1 \, dx = \frac{1}{3}\int_D \nabla \cdot x \, dx = \frac{1}{3}\int_{\partial D} x \cdot \nu \, do = \frac{1}{3}\int_\Gamma id_\Gamma \cdot \nu \, do.$$

The assumption of a fixed enclosed volume can hence be written as $V(\Gamma) = V_0$, where

$$V(\Gamma) := \frac{1}{3}\int_\Gamma id_\Gamma \cdot \nu \, do.$$

We introduce this constraint into the energy functional via a Lagrange multiplier. This yields to the following Lagrangian functional which will be the principal object of our study in this section

$$\mathcal{L}(\Gamma,\lambda) := \int_\Gamma \frac{1}{2}\kappa H^2 + \sigma \, do + \lambda\left(V(\Gamma) - V_0\right). \tag{4.17}$$

Remark 4.3.1. *In the variational formulation the term associated with the Lagrange multiplier λ corresponds to a constraining force, which in the above case can be interpreted as a hydrostatic pressure maintaining the volume constant.*

In this section we will consider a critical point for the Lagrangian $\mathcal{L}$, which we will denote by (Γ_0, λ_0). This means that (Γ_0, λ_0) satisfies

$$\begin{cases} \left.\dfrac{d}{ds}\mathcal{L}(\Gamma_0, \lambda_0 + s\mu)\right|_{s=0} = 0, & \forall \mu \in \mathbb{R}, \\ \left.\dfrac{d}{ds}\mathcal{L}(\Gamma_s, \lambda_0)\right|_{s=0} = 0, & \forall u \in C^2(\Gamma_0), \end{cases} \tag{4.18}$$

where $\Gamma_s := \{p + s(u\nu)(p) \mid p \in \Gamma_0\}$. We will refer to Γ_0 as an undeformed surface. As for the tensionless membrane we will consider small deformations that are due to some small external forces. They will be incorporated into this model by perturbing the Lagrangian.

4.3.1 Deformations due to small external forces

As for the tensionless membrane we consider arbitrary small forces $\varepsilon\mathcal{F}$ which give rise to deformed surfaces of the form Γ_ε as given in (4.7). We also assume it is possible to write the Lagrange multiplier associated with the deformed membrane as $\lambda_\varepsilon = \lambda_0 + \varepsilon\mu$ for some $\mu \in \mathbb{R}$. The perturbed Lagrangian is hence given by

$$\mathcal{L}_\varepsilon(\Gamma_\varepsilon, \lambda_\varepsilon) := \mathcal{W}(\Gamma_\varepsilon) + \lambda_\varepsilon(V(\Gamma_\varepsilon) - V(\Gamma_0)) - \varepsilon\mathcal{F}(\Gamma_\varepsilon). \tag{4.19}$$

We are motivated by attempting to find critical points of this energy. The rationale for this is that if Γ_ε minimises the perturbed Helfrich energy

$$\mathcal{W}(\Gamma_\varepsilon) - \varepsilon\mathcal{F}(\Gamma_\varepsilon),$$

subject to the volume constraint $V(\Gamma_\varepsilon) = V(\Gamma_0)$, then there exists a $\lambda_\varepsilon \in \mathbb{R}$ such that $(\Gamma_\varepsilon, \lambda_\varepsilon)$ is a critical point for $\mathcal{L}_\varepsilon$. Similarly to the construction of J in the tensionless case, we aim to find a good approximation for this Lagrangian for which the determination of critical points reduces to a linear PDE. To do so we perform a second order Taylor expansion in ε, using a slight abuse of notation $\mathcal{L}_\varepsilon(u, \mu) = \mathcal{L}_\varepsilon(\Gamma_\varepsilon, \lambda_\varepsilon)$.

$$\mathcal{L}_\varepsilon(u,\mu) = \mathcal{L}_0(u,\mu) + \varepsilon \frac{\mathrm{d}\mathcal{L}_\varepsilon(u,\mu)}{\mathrm{d}\varepsilon}\bigg|_{\varepsilon=0} + \frac{\varepsilon^2}{2}\frac{\mathrm{d}^2\mathcal{L}_\varepsilon(u,\mu)}{\mathrm{d}\varepsilon^2}\bigg|_{\varepsilon=0} + O(\varepsilon^3). \tag{4.20}$$

We observe that the first term $\mathcal{L}_0(u,\mu) = \mathcal{W}(\Gamma_0)$ does not depend on u or μ. Since (Γ_0, λ_0) is assumed to be a critical point of $\mathcal{L}$, the second term reduces to $-\mathcal{F}(\Gamma_0)$ and thus does not depend on u or μ. We therefore see that the lowest order term that depends on u or μ is the second order term. The Taylor expansion hence can be written as

$$\mathcal{L}(u,\mu) = \mathcal{W}(\Gamma_0) - \varepsilon\mathcal{F}(\Gamma_0) + \varepsilon^2 L(u,\mu) + O(\varepsilon^3),$$

with

$$L(u,\mu) := \frac{1}{2}\frac{\mathrm{d}^2\mathcal{L}_\varepsilon(u,\mu)}{\mathrm{d}\varepsilon^2}\bigg|_{\varepsilon=0}. \tag{4.21}$$

The approximate Lagrangian $L(u,\mu)$ is the sum of variations of the functionals $\mathcal{W}$, V and $\mathcal{F}$. To derive an explicit formula for $L(u,\mu)$ will be part of the next section. Instead of determining critical points of the original Lagrangian in (4.19), we aim to approximate them by considering the novel Lagrangian L.

4.3.2 Derivation of a Lagrangian for the height function

Similarly to the treatment of J in the tensionless case we calculate L in terms of variations of its constituent functionals. The second variation of $\mathcal{W}$ is calculated by combining the second variations of the Willmore functional W and the area functional A, both given in the appendix. We take derivatives of the force term involving $\mathcal{F}$ as previously and also require variations of the volume functional V which are also computed in the appendix. The functional L is a novel quadratic Lagrangian with which we will formulate the variational problems related to surface displacement.

Definition 4.3.1. *For the surface $\Gamma_0 \subset \mathbb{R}^3$ with associated Lagrange multiplier*

$\lambda_0 \in \mathbb{R}$, *the quadratic surface Lagrangian* $L : H^2(\Gamma_0) \times \mathbb{R} \to \mathbb{R}$ *is given by*

$$\begin{aligned} L(u,\mu) :&= \frac{1}{2}\frac{\mathrm{d}^2\mathcal{L}_\varepsilon(u)}{\mathrm{d}\varepsilon^2}\bigg|_{\varepsilon=0}, \\ &= \frac{1}{2}\mathcal{W}''(\Gamma_0)[u\nu,u\nu] + \frac{1}{2}\lambda_0 V''(\Gamma_0)[u\nu,u\nu] + \mu V'(\Gamma_0)[u\nu] - \mathcal{F}'(\Gamma_0)[u]. \end{aligned}$$

Under the assumption that (Γ_0, λ_0) is chosen such that the first variation $\mathcal{L}'(\Gamma_0, \lambda_0)$ vanishes, by the Taylor expansion (4.20), $L(u,\mu)$ is an $O(\varepsilon^3)$ order approximation of $\mathcal{L}_\varepsilon(u,\mu)$, up to an additive constant. Henceforward, we will neglect the terms which do not depend on u or μ and the $O(\varepsilon^3)$ terms. In this case the only undeformed surface we consider is a sphere, $\Gamma_0 = S(0,R)$. It follows

$$\frac{d}{ds}\mathcal{L}(\Gamma_s, \lambda_0) = \int_{\Gamma_0} \sigma H u + \lambda_0 u,$$

hence fixing the Lagrange multiplier $\lambda_0 = -\sigma H = -2\sigma/R$ ensures that (4.18) is satisfied. The linearised Lagrangian is given explicitly by

$$L(u,\mu) = \frac{1}{2}\int_{\Gamma_0} \kappa(\Delta_{\Gamma_0}u)^2 + \left(\sigma - \frac{2\kappa}{R^2}\right)|\nabla_{\Gamma_0}u|^2 - \frac{2\sigma}{R^2}u^2 + 2\mu u \, do - \mathcal{F}'(\Gamma_0)[u].$$

Similarly to the tensionless case, it is important to identify a subspace of $H^2(\Gamma_0)$ over which the bilinear form corresponding to the quadratic part of the Lagrangian is coercive. In this case the appropriate bilinear form is given by

$$a_\sigma(u,v) := \int_{\Gamma_0} \kappa\Delta_{\Gamma_0}u\Delta_{\Gamma_0}v + \left(\sigma - \frac{2\kappa}{R^2}\right)\nabla_{\Gamma_0}u \cdot \nabla_{\Gamma_0}v - \frac{2\sigma}{R^2}uv \, do. \tag{4.22}$$

Notice that a_σ is coercive over $Ker(a)^\perp$, where $Ker(a) = sp\{1, \nu_1, \nu_2, \nu_3\}$, again we refer to orthogonality with respect to the $H^2(\Gamma_0)$ inner product but recall this is equivalent to orthogonality with respect to the $L^2(\Gamma_0)$ inner product in this case (see (4.16)). Furthermore, $Ker(a)^\perp$ is the largest subspace of $H^2(\Gamma_0)$ over which it is coercive. Notice also that on such a subspace the term associated with the linearised Lagrange multiplier vanishes

$$\int_{\Gamma_0} 2\mu u \, do = 0 \quad \text{for all } (u,\mu) \in Ker(a)^\perp \times \mathbb{R}.$$

We can thus pose variational problems in precisely the same manner for the tensionless case and for membranes under tension, simply by using the bilinear form a or a_σ as appropriate and working over the space $Ker(a)^\perp$. Studying such variational problems will be the subject of the next section.

4.4 Minimising the linearised Willmore functional with point forces and point displacement constraints

In this section we will take the undeformed surface to be a sphere, $\Gamma = S(0, R)$, or a Clifford torus $\Gamma = T(R, R\sqrt{2})$. However for problems involving surface tension, that is $\sigma > 0$, we will only consider a sphere $\Gamma = S(0, R)$. Note we drop the subscript for the undeformed surfaces, simply referring to them as Γ. As done for the flat case, see Chapter 2, we may study the interactions of the membrane with thin filaments. These filaments are anchored to the cytoskeleton. Their effects are modelled by applying a point force or point constraint to the membrane. We begin with point forces.

4.4.1 Point forces

We begin by studying the effect of point forces applied in the normal direction to Γ. We will consider N point forces at locations $X_1, ..., X_N \in \Gamma$, which we will henceforth denote by $X := (X_1, ..., X_N) \in \Gamma^N$. We use a functional $\mathcal{F}_X$ in (4.6) giving rise to $\mathcal{F}'_X(\Gamma)$, such that

$$\mathcal{F}'_X(\Gamma)[u] := \sum_{i=1}^{N} \beta_i u(X_i). \tag{4.23}$$

Here $\beta_i \in \mathbb{R} \setminus \{0\}$ are constants related to the magnitudes of the forces, hence the force term measures the work done by the point forces. To emphasise the dependence of the resulting quadratic energy functional J upon the locations of the point forces X we will use the notation $\mathcal{E} : H^2(\Gamma) \times \Gamma^N \to \mathbb{R}$ defined by

$$\mathcal{E}(u, X) := \frac{1}{2} a_\sigma(u, u) - \mathcal{F}'_X(\Gamma)[u].$$

Here a_σ is the bilinear functional defined in (4.22) for $\sigma > 0$ and the second variation of the Willmore functional, defined in (4.13), for $\sigma = 0$. In light of the previous two sections, to formulate a well posed minimisation for $\mathcal{E}(\cdot, X)$ problem we work over the linear space

$$V := Ker(a)^\perp = \left\{ v \in H^2(\Gamma) \mid (v, w)_{H^2(\Gamma)} = 0 \; \forall w \in Ker(a) \right\}.$$

Here $Ker(a)$, which depends upon the choice of undeformed surface Γ, is constructed as in Lemma 4.2.2. Note that we could attempt to pose a minimisation problem over the whole space $H^2(\Gamma)$ but this would need a compatibility condition on the linear functional $\mathcal{F}'_X$ for existence and constraints on u for uniqueness. We now state the energy minimisation problem and give an equivalent variational form.

Problem 4.4.1 (Point forces at fixed locations).
For given $X \in \Gamma^N$ find $u_X \in V$ satisfying the two equivalent properties

(a) u_X minimises $\mathcal{E}(\cdot, X)$ on V,

(b) $a_\sigma(u_X, v) = \sum_{k=1}^N \beta_k v(X_k)$ for all $v \in V$.

Existence and uniqueness of a solution to this problem follows from the Lax-Milgram theorem. Note, for a sphere the projection out of $Ker(a)$ can be justified physically. The minimisation problem above has a corresponding PDE representation involving four Lagrange multipliers, as $Ker(a) = Sp\{1, \nu_1, \nu_2, \nu_3\}$ is four dimensional for a sphere. The Lagrange multiplier associated with the constant function 1 corresponds to a linearised hydrostatic pressure which enforces the volume constraint. Each of the three remaining Lagrange multipliers is associated with one of the components of the normal ν_i. It can be shown that these multipliers correspond to linearised reaction forces which prevent $O(\varepsilon)$ translations of the centre of mass of the domain D enclosed by Γ.

We also consider varying the locations $X \in \Gamma^N$, this problem can be stated in two equivalent forms.

Problem 4.4.2 (Point forces with varying locations).

(a) Find $(u, X) \in V \times \Gamma^N$ minimising the energy $\mathcal{E}(\cdot, \cdot)$ on $V \times \Gamma^N$.

(b) Find $X \in \Gamma^N$ minimising the energy $X \mapsto \mathcal{E}(u_X, X)$ on Γ^N.

Existence of solutions for (a) follows by the same general theory that was applied in the flat case, see Proposition A.1.3. Note (a) and (b) are equivalent in the sense that (u, X) solves (a) if and only if X solves (b) and $u = u_X$. We will thus refer to these equivalent minimisation problems simply as Problem 4.4.2.

Proposition 4.4.1. *Without loss of generality assume $\beta_1 \leq \beta_2 \leq ... \leq \beta_N$.*

Suppose $\boldsymbol{\beta_1 > 0}$ or $\boldsymbol{\beta_N < 0}$.

$X \in \Gamma^N$ solves Problem 4.4.2 if and only if $X_i = X_0$ for all $i = 1, ..., N$ where $X_0 \in \Gamma$ is a solution to Problem 4.4.2 with parameters $\tilde{N} = 1$ and $\tilde{\beta_1} = \sum_{i=1}^N \beta_i$.

Suppose $\boldsymbol{\beta_k < 0}$ and $\boldsymbol{\beta_{k+1} > 0}$ for some $\boldsymbol{1 \leq k \leq N - 1}$.

$X \in \Gamma^N$ solves Problem 4.4.2 if and only if both of the following hold.

1. $X_i = X^-$ *for all* $i = 1, ..., k$ *and* $X_i = X^+$ *for all* $i = k+1, ..., N$.
2. $(X^+, X^-) \in \Gamma^2$ *solves Problem 4.4.2 with parameters* $\tilde{N} = 2$ *and* $\tilde{\beta} = \left(\sum_{i=1}^{k} \beta_i, \sum_{i=k+1}^{N} \beta_i\right)$.

Proof. For $y \in \Gamma$, let ϕ_y denote the solution to Problem 4.4.1 with $N = 1$, $X = (y)$ and $\beta_1 = 1$. By linearity it follows, for any $X \in \Gamma^N$,

$$u_X = \sum_{i=1}^{N} \beta_j \phi_{X_i}.$$

To prove the first statement, suppose $X_0 \in \Gamma$ is a solution to Problem 4.4.2 with parameters $\tilde{N} = 1$ and $\tilde{\beta}_1 = 1$. Note that we have assumed $sign(\beta_1) = ... = sign(\beta_N)$, hence for any $X \in \Gamma^N$,

$$\begin{aligned}
\mathcal{E}(u_X, X) &= -\frac{1}{2} \sum_{i,j=1}^{N} \beta_i \beta_j a_\sigma(\phi_{X_i}, \phi_{X_j}) \\
&\geq -\frac{1}{2} \sum_{i,j=1}^{N} \beta_i \beta_j a_\sigma(\phi_{X_i}, \phi_{X_i})^{1/2} a_\sigma(\phi_{X_j}, \phi_{X_j})^{1/2} \\
&\geq -\frac{1}{2} \sum_{i,j=1}^{N} \beta_i \beta_j a_\sigma(\phi_{X_0}, \phi_{X_0}) = \mathcal{E}(u_{\tilde{X}}, \tilde{X})
\end{aligned}$$

where $\tilde{X} = (X_0, ..., X_0)$. The first inequality used is the Cauchy Schwarz inequality and the second inequality follows from the definition of X_0. As these inequalities hold for any $X \in \Gamma^N$ we have proven the backwards implication.

Now suppose $X \in \Gamma^N$ solves Problem 4.4.2, then in addition to the inequalities derived above it holds

$$\mathcal{E}(u_{\tilde{X}}, \tilde{X}) \geq \mathcal{E}(u_X, X),$$

hence equality holds at each step. Then, as we have equality in the Cauchy Schwarz inequalities used, ϕ_{X_i} and ϕ_{X_j} are linearly dependent for each i, j. It follows $X_1 = X_2 = ... = X_N$ and for any $y \in \Gamma$, set $Y = (y, y, ..., y) \in \Gamma^N$ then

$$-\frac{1}{2} \sum_{i,j=1}^{N} \beta_i \beta_j a_\sigma(\phi_y, \phi_y) = \mathcal{E}(u_Y, Y) \geq \mathcal{E}(u_X, X) = -\frac{1}{2} \sum_{i,j=1}^{N} \beta_i \beta_j a_\sigma(\phi_{X_1}, \phi_{X_1}).$$

Hence $X_1 \in \Gamma$ is a solution to Problem 4.4.2 with parameters $\tilde{N} = 1$ and $\tilde{\beta}_1 = 1$ and we have proven the forwards implication.

For the second statement observe, for any $Y, Z \in \Gamma^N$,

$$\begin{aligned}\mathcal{E}(u_Y, Y) &= \mathcal{E}(u_Z, Z) - a_\sigma(u_Y - u_Z, u_Z) - \frac{1}{2} a_\sigma(u_Y - u_Z, u_Y - u_Z), \\ &= \mathcal{E}(u_Z, Z) - \sum_{i=1}^{N} \beta_i (u_Z(Y_i) - u_Z(Z_i)) - \frac{1}{2} a_\sigma(u_Y - u_Z, u_Y - u_Z).\end{aligned}$$

Now suppose $X \in \Gamma^N$ solves Problem 4.4.2 and there exists $1 \leq i < j \leq k$ such that $X_i \neq X_j$. Without loss of generality assume $u_X(X_j) \leq u_X(X_i)$. Let $X' \in \Gamma^N$ be given by $X'_l = X_l$ for $l \neq i$ and $X'_i = X_j$. Then using the above calculation we obtain

$$\mathcal{E}(u_{X'}, X') = \mathcal{E}(u_X, X) - \beta_i (u_X(X_j) - u_X(X_i)) - \frac{1}{2} a_\sigma(u_{X'} - u_X, u_{X'} - u_X). \tag{4.24}$$

As $X \neq X'$ it follows $u_X \neq u_{X'}$ and hence $a_\sigma(u_{X'} - u_X, u_{X'} - u_X) > 0$. Thus

$$\mathcal{E}(u_{X'}, X') < \mathcal{E}(u_X, X)$$

which is a contradiction, hence $X_1 = X_2 = ... = X_k =: X^-$. An identical argument shows $X_{k+1} = X_{k+2} = ... = X_N =: X^+$. It follows

$$u_X = \sum_{l=1}^{k} \beta_l \phi_{X^-} + \sum_{l=k+1}^{N} \beta_l \phi_{X^+}.$$

Now for any $(Y^+, Y^-) \in \Gamma^2$ let $Y \in \Gamma^N$ be such that $Y_l = Y^-$ for $1 \leq l \leq k$ and $Y_l = Y^+$ for $k+1 \leq l \leq N$. Then $\mathcal{E}(u_X, X) \leq \mathcal{E}(u_Y, Y)$ and using the above expression for u_X we deduce that (X^+, X^-) solves Problem 4.4.2 with parameters $\tilde{N} = 2$ and $\tilde{\beta} = \left(\sum_{i=1}^{k} \beta_i, \sum_{i=k+1}^{N} \beta_i\right)$.

For the reverse implication in the second statement, suppose $Y \in \Gamma^N$. Using the same technique as in (4.24) we may form $Y' \in \Gamma^N$ such that $Y'_1 = ... = Y'_k$, $Y'_{k+1} = ... = Y'_N$ and $\mathcal{E}(u_{Y'}, Y') \leq \mathcal{E}(u_Y, Y)$. Then, using the fact that (X^+, X^-) solves the $N = 2$ problem,

$$\mathcal{E}(u_X, X) \leq \mathcal{E}(u_{Y'}, Y') \leq \mathcal{E}(u_Y, Y).$$

Hence X solves Problem 4.4.2. □

Note there is no uniqueness for this problem in general. Indeed, for the problem on a sphere with $N = 1$, every $X \in S(0, R)$ solves Problem 4.4.2 due to rotational symmetry.

4.4.2 Point value constraints

We will now consider filaments which fix the location of the membrane at a point. To do so we consider the following perturbed energy functional, for a general surface $\tilde{\Gamma}$,

$$\mathcal{W}_\delta(\tilde{\Gamma}) := \mathcal{W}(\tilde{\Gamma}) + \frac{1}{2\delta}\sum_{i=1}^{N} d(\tilde{\Gamma}, y_i)^2.$$

Here $\delta > 0$ is a small penalty parameter, d denotes the signed distance to the surface $\tilde{\Gamma}$ and $y_1, ..., y_N \in \mathbb{R}^3$ are the locations fixed by the filaments. Similarly to the point forces, we assume the additional term is a small perturbation to the Willmore functional so that the resulting deformed surface may be expressed in the form Γ_ε, a graph over the undeformed surface Γ, which is chosen to be a sphere or Clifford torus here. In this case the small perturbation assumption is justified when the locations y_i can be expressed in the form

$$y_i = X_i + \varepsilon\alpha_i\nu(X_i), \tag{4.25}$$

for some $X \in \Gamma^N$ and $\alpha \in \mathbb{R}^N$. As ν is determined by the choice of undeformed surface Γ and of unit length, it is equivalent to see this as a penalty method for u, the height function. Note that we could also formulate a similar problem without the penalty method by applying point constraints to the displacement u.

The first problem we consider is for fixed locations. We begin by stating the general, non-linear problem which we aim to approximate.

Problem 4.4.3 (Point value constraints for W)**.**
Given $X \in \Gamma^N$, $\alpha \in \mathbb{R}^N$ and $\delta > 0$, find $u \in H^2(\Gamma)$ minimising $\mathcal{W}_\delta(\Gamma_\varepsilon(u))$.

That is we wish to find the surface of the form $\Gamma_\varepsilon(u) = \{p + \varepsilon(u\nu)(p) \mid p \in \Gamma\}$ which minimises the penalised Willmore energy $\mathcal{W}_\delta$. For a surface of the form Γ_ε, with the small perturbation assumption (4.25), this energy reads

$$\mathcal{W}_\delta(\Gamma_\varepsilon) = \mathcal{W}(\Gamma_\varepsilon) + \frac{1}{2\delta}\sum_{i=1}^{N} d(\Gamma_\varepsilon, X_i + \varepsilon\alpha_i\nu(X_i))^2.$$

We will use $(\varepsilon^2/2)a_\sigma(\cdot,\cdot)$, the previously defined second order approximation to $\mathcal{W}(\Gamma_\varepsilon)$. We require a similar approximation of the distance function term. First notice

$$d(\Gamma_\varepsilon, X_i + \varepsilon\alpha_i\nu(X_i))\big|_{\varepsilon=0} = d(\Gamma, X_i) = 0.$$

Secondly, the first derivative with respect to ε is given by

$$\begin{aligned}\frac{d}{d\varepsilon}d(\Gamma_\varepsilon, X_i + \varepsilon\alpha_i\nu(X_i))\bigg|_{\varepsilon=0} &= \nabla d(\Gamma, X_i)\cdot\frac{d}{d\varepsilon}(X_i + \varepsilon\alpha_i\nu(X_i))\bigg|_{\varepsilon=0} + \dot{\partial} d(\Gamma_\varepsilon, X_i),\\ &= \alpha_i - u(X_i).\end{aligned}$$

The final line holds as $\nabla d(\Gamma, X_i) = \nu(X_i)$ and $\dot{\partial} d(\Gamma_\varepsilon, X_i) = -u(X_i)$, see [42]. It follows, expanding in ε as previously,

$$d(\Gamma_\varepsilon, X_i + \varepsilon\alpha_i\nu(X_i))^2 = \varepsilon^2(u(X_i) - \alpha_i)^2 + O(\varepsilon^3).$$

We thus minimise the penalised quadratic energy functional

$$J_\delta(u) := \frac{1}{2}a_\sigma(u,u) + \frac{1}{2\delta}\sum_{i=1}^{N}(u(X_i) - \alpha_i)^2.$$

When $\sigma > 0$ this functional is minimised subject to the constraint $\int_\Gamma u\ do = 0$, which is the linearised form of the fixed volume constraint.

Similarly to the point forces problem this minimisation is not well posed over $H^2(\Gamma)$ and we must identify an appropriate subspace over which the problem is well posed. In order to identify an appropriate subspace we first introduce the following notation for affine subspaces.

Definition 4.4.1. *Suppose $Z \subset H^2(\Gamma)$ is a linear subspace, $X \in \Gamma^N$ and $\gamma \in \mathbb{R}^N$. We denote by $Z_{X,\gamma}$ the affine space given as follows,*

$$Z_{X,\gamma} := \{z \in Z \mid z(X_i) = \gamma_i \ \forall i = 1, ..., N\}.$$

For the linearised problem we consider the space $U_\sigma \subset H^2(\Gamma)$ given by

$$U_\sigma := \begin{cases} \left(H^2_{X,0}(\Gamma)\cap Ker(a)\right)^\perp & \text{if } \sigma = 0,\\ \left\{u \in \left(H^2_{X,0}(\Gamma)\cap Ker(a)\right)^\perp \mid \int_\Gamma u\ do = 0\right\} & \text{if } \sigma > 0.\end{cases}$$

Here $\perp$ again means orthogonality with respect to the H^2 inner product. In the $\sigma = 0$ case, the space U_σ is the largest subspace of $H^2(\Gamma)$ over which well-posedness is possible. If we used a larger subspace $Z \supset U_\sigma$ then there exist elements $0 \neq v_0 \in Z \cap \left(H^2_{X,0}(\Gamma)\cap Ker(a)\right)$. For such elements $J_\delta(u + v_0) = J_\delta(u)$ hence no uniqueness is possible. A similar argument shows U_σ is the largest subspace of $\left\{u \in H^2(\Gamma) \mid \int_\Gamma u\ do = 0\right\}$ over which well-posedness is possible in the $\sigma > 0$ case.

Remark 4.4.1. *Notice that $Ker(a)$ is a finite dimensional space and $u \in H^2_{X,0}(\Gamma)$ satisfies N conditions of the form $u(X_i) = 0$. The generic case for $N > dim(Ker(a))$ is thus $H^2_{X,0}(\Gamma) \cap Ker(a) = \{0\}$, producing U_σ such that*

$$U_\sigma := \begin{cases} H^2(\Gamma) & \text{if } \sigma = 0, \\ \left\{u \in H^2(\Gamma) \;\middle|\; \int_\Gamma u \, do = 0\right\} & \text{if } \sigma > 0. \end{cases}$$

We now state the quadratic minimisation problem that will be studied.

Problem 4.4.4. *Given $X \in \Gamma^N$, $\alpha \in \mathbb{R}^N$ and $\delta > 0$ find $u_\delta \in U_\sigma$ minimising J_δ over U_σ.*

Proposition 4.4.2. *For each $\delta > 0$ there exists a unique solution u_δ to Problem 4.4.4.*

Proof. Define a bilinear form $a^\delta_\sigma : U_\sigma \times U_\sigma \to \mathbb{R}$ by

$$a^\delta_\sigma(u, v) := a_\sigma(u, v) + \frac{1}{\delta} \sum_{i=1}^{N} u(X_i) v(X_i).$$

Notice a^δ_σ is bounded, symmetric and positive semi-definite, hence weak lower semi-continuous. In fact it is also coercive, we prove this by contradiction. Assume a^δ_σ is not coercive over U_σ, then there exists a sequence $u_n \in U_\sigma$ such that

$$\|u_n\|_{H^2(\Gamma)} = 1 \text{ and } a^\delta_\sigma(u_n, u_n) < \frac{1}{n} \text{ for all } n \geq 1.$$

Then we may find a subsequence $u_{n'} \rightharpoonup u$ for some $u \in U_\sigma$, it follows

$$0 \leq a^\delta_\sigma(u, u) \leq \lim_{n' \to \infty} a^\delta_\sigma(u_{n'}, u_{n'}) = 0.$$

Thus $u \in U_\sigma \cap Ker(a^\delta_\sigma) = U_\sigma \cap (H^2_{X,0}(\Gamma) \cap Ker(a)) = \{0\}$. Now for each n', $u_{n'}$ may be expressed uniquely in the form

$$u_{n'} = p_{n'} + q_{n'} \text{ with } p_{n'} \in Ker(a)^\perp \text{ and } q_{n'} \in Ker(a).$$

The bilinear form a_σ is coercive over $Ker(a)^\perp$, hence

$$C\|p_{n'}\|^2_{H^2(\Gamma)} \leq a_\sigma(p_{n'}, p_{n'}) = a_\sigma(u_{n'}, u_{n'}) \leq a^\delta_\sigma(u_{n'}, u_{n'}) \to 0,$$

thus $p_{n'} \to 0$. It follows that $q_{n'} \rightharpoonup 0$ and thus $q_{n'} \to 0$ as $Ker(a)$ is finite dimensional. We have reached a contradiction as now it holds that

$$1 = \|u_{n'}\|^2_{H^2(\Gamma)} = \|p_{n'}\|^2_{H^2(\Gamma)} + \|q_{n'}\|^2_{H^2(\Gamma)} \to 0.$$

Hence there exists $\gamma > 0$ such that

$$\gamma \|u\|^2_{H^2(\Gamma)} \leq a^\delta_\sigma(u,u) \quad \forall u \in U_\sigma.$$

Now write J_δ in the form

$$J_\delta(u) = \frac{1}{2} a^\delta_\sigma(u,u) - \frac{1}{\delta}\sum_{i=1}^N \alpha_i u(X_i) + \frac{1}{2\delta}\sum_{i=1}^N \alpha_i^2.$$

The existence of a unique solution to Problem 4.4.4 is then a consequence of the Lax-Milgram theorem. □

We now state the limit problem which solutions to Problem 4.4.4, u_δ, converge to as $\delta \downarrow 0$, first we introduce the notion of prescribed point values.

Prescribed point values at distinct locations $X = (X_i) \in \Gamma^N$ will be represented by the constraints

$$F_X(u) = \alpha \tag{4.26}$$

with given $\alpha \in \mathbb{R}^N$ and F_X defined by

$$F_X(u) = (u(X_1), ..., u(X_N)) \in \mathbb{R}^N. \tag{4.27}$$

Note that this is well defined as the map $u \mapsto u(X_i) \in H^2(\Gamma)^*$ due to the continuous embedding $H^2(\Gamma) \subset C(\Gamma)$ (see [3, Theorem 2.20]). With this concept of prescribed point values we can state the limit problem.

Problem 4.4.5 (Point value constraints)**.**
Find $u \in (U_\sigma)_{X,\alpha}$ satisfying the following equivalent conditions.

1. *$u \in (U_\sigma)_{X,\alpha}$ minimises $u \mapsto \frac{1}{2}a_\sigma(u,u)$ over $(U_\sigma)_{X,\alpha}$.*
2. *$u \in (U_\sigma)_{X,\alpha}$ is such that $a_\sigma(u,v) = 0$ for all $v \in (U_\sigma)_{X,0}$.*

Existence and uniqueness of a solution to this problem follows from the fact that $a_\sigma(\cdot,\cdot)$ is coercive over $(U_\sigma)_{X,0}$, which is deduced from the observation $a^\delta_\sigma(v,v) = a_\sigma(v,v)$ for $v \in (U_\sigma)_{X,0}$, as a^δ_σ is coercive over U_σ, shown in the proof of Proposition 4.4.2. We now show convergence for the penalty method.

Proposition 4.4.3. *For $\delta > 0$ let u_δ denote the unique solution of Problem 4.4.4 and u the unique solution of Problem 4.4.5, then $u_\delta \to u$ in $H^2(\Gamma)$-norm as $\delta \downarrow 0$.*

For a proof see Proposition A.2.1.

A natural question to consider is minimising over the constraint locations X as well as the displacement u, analogous to Problem 4.4.2. The general theory in Appendix A is used in Chapter 2 to establish a minimum for this type of problem, when the constraint locations X are allowed to vary in the planar case. This theory cannot be applied here however as the underlying Hilbert space U_σ depends upon the locations X.

4.5 Second order splitting method

The equivalent PDEs to the point forces and point constraints problems are fourth order and their weak formulations are posed in subspaces of $H^2(\Gamma)$. To produce a finite element method which directly solves these problems therefore requires some H^2-conforming element or some suitable non-conforming element. This approach is not taken here, instead we will formulate a second order splitting for our problems. This will turn the fourth order PDE into a system of second order PDEs which we may solve with standard piecewise linear finite elements. In our numerical examples we will investigate point forces on a sphere and point constraints on a torus. We will first present the splitting method and finite element analysis for the problem on the sphere. The problem on the torus falls in to a broader class which will be analysed in Chapter 5.

For clarity we now state the variational form of the point forces problem upon which the splitting method is based. In this section we set $\Gamma = S(0, R)$, a sphere of radius R.

Problem 4.5.1. *Find $u \in V$ such that*

$$a_\sigma(u, v) = \sum_{i=1}^{N} \beta_i v(X_i) \quad \forall v \in V.$$

We will enforce the constraint $u \in V = Ker(a)^\perp$ via the addition of a new bilinear form and an adjustment of the right hand side. For the numerical method we will express the condition $u \in V$ via $L^2(\Gamma)$-orthogonality. For each basis function of $Ker(a)$, f_i, set

$$g_i := (\Delta_\Gamma^2 - \Delta_\Gamma + 1) f_i \in C^\infty(\Gamma).$$

We can then characterise V in terms of $L^2(\Gamma)$-orthogonality with the g_i, for $1 \leq i \leq M := dim(Ker(a))$,

$$V = \left\{ v \in H^2(\Gamma) \mid (v, g_i)_{L^2(\Gamma)} = 0 \ \forall 1 \leq i \leq M \right\}.$$

Using the basis functions given in Lemma 4.2.2, for a sphere the g_i are given by

$$\left\{ 1, \left(\frac{4}{R^4} + \frac{2}{R^2} + 1 \right) \nu_i \ \middle| \ i = 1, 2, 3 \right\},$$

in our applications we will take the constant multiplying the ν_i to be 1, that is we take the basis $\{1, \nu_1, \nu_2, \nu_3\}$. Note that this basis is an $L^2(\Gamma)$-orthogonal set.

The variational problem is posed over V, a subspace of $H^2(\Gamma)$. For ease of implementation, we wish to solve a problem posed over the full space $H^2(\Gamma)$. To formulate such a problem we introduce Lagrange multipliers, the resulting variational problem is shown below.

Problem 4.5.2. *Find* $(u, \lambda) \in H^2(\Gamma) \times \mathbb{R}^4$ *such that*

$$a_\sigma(u, v) = \sum_{k=1}^{N} \beta_k v(X_k) - \lambda_0 \int_\Gamma v \, do - \sum_{i=1}^{3} \lambda_i \int_\Gamma v \nu_i \, do \quad \forall v \in H^2(\Gamma),$$
$$\int_\Gamma u \, do = \int_\Gamma u \nu_i \, do = 0 \quad \textit{for } i = 1, 2, 3.$$

By testing with $v \in V$ we see if (u, λ) solves Problem 4.5.2 then u solves Problem 4.5.1.

Here we can easily determine the Lagrange multipliers. Testing the first equation with a component of the normal, ν_i, or the constant function 1 we obtain zero on the left hand side, using $\int_\Gamma u \, do = 0$ for the latter case. The right hand side must likewise vanish, determining the Lagrange multipliers

$$\lambda_0 = \frac{1}{4\pi R^2} \sum_{k=1}^{N} \beta_k \quad \text{and} \quad \lambda_i = \frac{3}{4\pi R^2} \sum_{k=1}^{N} \beta_k \nu_i(X_k) \quad \text{for} \quad i = 1, 2, 3.$$

Now we have produced a problem for u which is posed over the full space $H^2(\Gamma)$ we can formulate the splitting method. To do so we will split this fourth order problem into a system of two second order equations. Such a splitting is best motivated by considering the strong form of Problem 4.5.2, produced by integrating the variational problem by parts,

$$
\begin{aligned}
\kappa\Delta_\Gamma^2 u - \left(\sigma - \frac{2\kappa}{R^2}\right)\Delta_\Gamma u - \frac{2\sigma}{R^2}u = \tilde{\delta}_X,& \\
\int_\Gamma u\, do = \int_\Gamma u\nu_i\, do = 0 \quad \text{for } i = 1,2,3.&
\end{aligned}
\tag{4.28}
$$

This equation is meant only in the sense of distributions, here $\tilde{\delta}_X$ denotes

$$
\tilde{\delta}_X := \sum_{k=1}^{N} \beta_k \left(\delta_{X_k} - \frac{1}{4\pi R^2} - \sum_{i=1}^{3} \frac{3}{4\pi R^2}\nu_i(X_k)\nu_i\right)
$$

where δ_{X_k} is the Dirac delta distribution $\delta_{X_k} : v \mapsto v(X_k)$. The PDE can also be given meaning in the sense that both sides lie in $H^2(\Gamma)^*$, this leads to the variational problem above.

To solve (4.28) numerically we will use a splitting method to formulate this fourth order problem as a pair of second order equations. The splitting occurs by introducing the new variable w, which satisfies

$$
w = -\Delta_\Gamma u - \frac{2}{R^2}u,
$$

it is immediate that w must satisfy the constraints

$$
\int_\Gamma w\, do = \int_\Gamma w\nu_i\, do = 0 \quad \text{for } i = 1,2,3.
$$

Using this splitting we are left with a decoupled system with constraints, given by

$$
\begin{aligned}
-\kappa\Delta_\Gamma w + \sigma w &= \tilde{\delta}_X, \\
-\Delta_\Gamma u - \frac{2}{R^2}u &= w, \\
\int_\Gamma w\, do &= 0 \quad \text{if } \sigma = 0, \\
\int_\Gamma u\nu_i\, do &= 0 \quad \text{for } i = 1,2,3.
\end{aligned}
\tag{4.29}
$$

The remaining properties

$$
\int_\Gamma u\, do = \int_\Gamma w\nu_i\, do = 0
$$

must hold for any solution of (4.29) hence need not be applied as constraints for this problem. Similarly, when $\sigma > 0$ the property

$$\int_\Gamma w \; do = 0$$

follows immediately from the first equation as $\langle \tilde{\delta}_X, 1\rangle = 0$.

We wish to find a weak formulation for this decoupled system to base our numerical method around. In addition, the implementation of the numerical method is much more straightforward if we can make the constraints a property of the equations we solve. Moreover, the problem is simpler to solve numerically if the operators on the left hand side of each equation satisfy an appropriate form of coercivity. We thus make a modification to the decoupled system, the modified system reads

$$\begin{aligned} -\kappa\Delta_\Gamma w + \sigma w + \chi_\sigma \int_\Gamma w &= \tilde{\delta}_X, \\ -\Delta_\Gamma u - \frac{2}{R^2}u + \tau \sum_{i=1}^{4} \left(\int_\Gamma u g_i \right) g_i &= w, \end{aligned}$$

where $\tau > 1/(2\pi R^4)$ and $\chi_\sigma = 1$ if $\sigma = 0$ and is zero otherwise. These choices are made to ensure coercivity of the resulting bilinear forms over $H^1(\Gamma)$. As $u, w \in V$ we have actually added zero to both equations but in doing so we ensure coercivity and that any solution to this modified system must satisfy the required constraints. We now give an appropriate weak formulation which will be discretised to produce the finite element method.

Problem 4.5.3. *Fix $X \in \Gamma^N$, $p \in (1,2)$ and $q \in (2,\infty)$ such that $1/p + 1/q = 1$. Find $(u,w) \in H^1(\Gamma) \times W^{1,p}(\Gamma)$ such that*

$$\int_\Gamma \kappa \nabla_\Gamma w \cdot \nabla_\Gamma v + \sigma w v \; do + \chi_\sigma (w,1)_{L^2(\Gamma)} (v,1)_{L^2(\Gamma)} = \langle \tilde{\delta}_X, v\rangle \qquad \forall v \in W^{1,q}(\Gamma),$$

$$\int_\Gamma \nabla_\Gamma u \cdot \nabla_\Gamma v - \frac{2}{R^2} uv \; do + \tau \sum_{i=1}^{4} (u,g_i)_{L^2(\Gamma)} (v,g_i)_{L^2(\Gamma)} = \int_\Gamma wv \; do \quad \forall v \in H^1(\Gamma).$$

This formulation is well posed and is equivalent to Problem 4.4.1 in the sense that the solution is given by $(u, -\Delta_\Gamma u - (2/R^2)u)$ where u is the solution to Problem 4.4.1. To establish this equivalence we begin with a weak formulation of the constrained system (4.29). The variational problem requires the following notation, for $W \subset L^2(\Gamma)$ we denote by W_σ and W_V the subsets

$$W_\sigma := \begin{cases} \left\{ v \in W \;\middle|\; \fint_\Gamma v \, do = 0 \right\} & \text{if } \sigma = 0, \\ W & \text{otherwise,} \end{cases}$$

$$W_V := \left\{ v \in W \;\middle|\; \int_\Gamma v \, do = \int_\Gamma v\nu_i \, do = 0 \text{ for } i = 1,2,3 \right\}.$$

Problem 4.5.4. *Fix $X \in \Gamma^N$, $p \in (1,2)$ and $q \in (2,\infty)$ such that $1/p + 1/q = 1$. Find $(w,u) \in W^{1,p}_V(\Gamma) \times H^1_V(\Gamma)$ such that*

$$\int_\Gamma \kappa \nabla_\Gamma w \cdot \nabla_\Gamma v + \sigma w v \, do = \langle \tilde{\delta}_X, v \rangle \qquad \forall v \in W^{1,q}_\sigma(\Gamma), \tag{4.30}$$

$$\int_\Gamma \nabla_\Gamma u \cdot \nabla_\Gamma v - \frac{2}{R^2} u v \, do = \int_\Gamma w v \, do \quad \forall v \in H^1_V(\Gamma). \tag{4.31}$$

Note that $W^{1,q}(\Gamma) \hookrightarrow C(\Gamma)$ so the right hand side in (4.30) is well defined. We now prove well posedness for this problem.

Proposition 4.5.1. *There exists a unique solution to Problem 4.5.4 and we have the improved regularity result $u \in W^{3,p}(\Gamma)$.*

Proof. We begin by solving (4.30). Define $T : L^2_\sigma(\Gamma) \to H^2_\sigma(\Gamma)$ by $Tf \in H^1_\sigma(\Gamma)$ the unique solution to

$$\int_\Gamma \kappa \nabla_\Gamma (Tf) \cdot \nabla_\Gamma v + \sigma (Tf) v = \int_\Gamma f v \quad \forall v \in H^1_\sigma(\Gamma).$$

Note by elliptic regularity $Tf \in H^2(\Gamma)$ so T is well defined and continuous. Thus consider the adjoint operator $T^* : H^2_\sigma(\Gamma)^* \to L^2_\sigma(\Gamma)$ and set $w := T^*(\tilde{\delta}_X) \in L^2_\sigma(\Gamma)$. Then for any $g \in L^2_\sigma(\Gamma)$ it holds

$$\int_\Gamma w g \, do = \langle T^*(\tilde{\delta}_X), g \rangle = \langle \tilde{\delta}_X, Tg \rangle.$$

Furthermore T is an isomorphism and for $v \in H^2_\sigma(\Gamma)$, $T^{-1} v = -\kappa \Delta_\Gamma v + \sigma v$. Thus for any $v \in H^2_\sigma(\Gamma)$

$$\int_\Gamma -\kappa w \Delta_\Gamma v + \sigma w v \, do = \int_\Gamma w T^{-1} v \, do = \langle \tilde{\delta}_X, v \rangle.$$

Now we will show $w \in W^{1,p}_V(\Gamma)$. First note $w \in L^2_\sigma(\Gamma) \hookrightarrow L^p_\sigma(\Gamma)$ and testing the above with $v = \nu_i$ and $v = 1$ if $\sigma \neq 0$ shows $w \in L^p_V(\Gamma)$. We now move to calculating the weak derivatives. We will use the following commutator rule, for $\phi \in C^3(\Gamma)$:

$$\underline{D}_\alpha \Delta_\Gamma \phi = \Delta_\Gamma \underline{D}_\alpha \phi + \frac{2}{R}\nu_\alpha \Delta_\Gamma \phi.$$

This follows from (4.1) applied to a sphere. Let $\phi \in C^1(\Gamma)$, $1 \leq \alpha \leq 3$ and $P : L^2(\Gamma) \to L^2_\sigma(\Gamma)$ denote the canonical projection onto $L^2_\sigma(\Gamma)$ (note this is simply the identity mapping if $\sigma > 0$) it follows

$$\begin{aligned}
\int_\Gamma w\underline{D}_\alpha \phi = \int_\Gamma w\underline{D}_\alpha P\phi = \int_\Gamma w\underline{D}_\alpha \left(-\kappa\Delta_\Gamma TP\phi + \sigma TP\phi\right), \\
= \int_\Gamma w\left(T^{-1}P(\underline{D}_\alpha TP\phi) - \frac{2\kappa}{R}\nu_\alpha\Delta_\Gamma TP\phi\right), \\
= \langle\tilde{\delta}_X, P(\underline{D}_\alpha TP\phi)\rangle + \int_\Gamma \frac{2}{R}w\nu_\alpha\left(P\phi - \sigma TP\phi\right).
\end{aligned}$$

Now consider the mapping $F_\alpha : L^q(\Gamma) \to \mathbb{R}$ given by

$$F_\alpha(\psi) := -\langle\tilde{\delta}_X, P(\underline{D}_\alpha TP\psi)\rangle + \int_\Gamma \frac{2\sigma}{R}w\nu_\alpha TP\psi.$$

Note, by elliptic regularity $T : L^q_V(\Gamma) \to W^{2,q}_V(\Gamma) \hookrightarrow C^1(\Gamma)$. Thus F_α is well defined and continuous, evidently it is also linear. Hence $F_\alpha \in L^q(\Gamma)^*$ and there exists $f_\alpha \in L^p(\Gamma)$ such that $F_\alpha = (f_\alpha, \cdot)$. It follows, for any $\phi \in C^1(\Gamma)$,

$$\int_\Gamma w\underline{D}_\alpha\phi = -\int_\Gamma f_\alpha\phi + \int_\Gamma Hw\phi\nu_\alpha.$$

Thus w is weakly differentiable with derivatives $\underline{D}_\alpha w = f_\alpha \in L^P(\Gamma)$ hence $w \in W^{1,p}_V(\Gamma)$. Furthermore, for any $v \in H^2_\sigma(\Gamma)$ it holds

$$\int_\Gamma \kappa\nabla_\Gamma w \cdot \nabla_\Gamma v + \sigma wv\, do = \int_\Gamma wT^{-1}v = \langle\tilde{\delta}_X, v\rangle.$$

As $H^2_\sigma(\Gamma)$ is dense in $W^{1,q}_\sigma(\Gamma)$ the above holds for $v \in W^{1,q}_\sigma(\Gamma)$ thus w is a solution to (4.30). For uniqueness, suppose w_1, w_2 solve (4.30). Then for any $v \in H^2_\sigma(\Gamma)$

$$\int_\Gamma (w_1 - w_2)T^{-1}v = 0.$$

The map T^{-1} maps $H^2_\sigma(\Gamma)$ onto $L^2_\sigma(\Gamma)$ thus $\|w_1 - w_2\|_{L^2(\Gamma)} = 0$ and the solution is unique.

For (4.31) observe that the choice of $H^1_V(\Gamma)$ projects out the eigenspace of the first two eigenvalues of $-\Delta_\Gamma$, hence we have the Poincaré inequality

$$\int_\Gamma v^2 \, do \leq \frac{6}{R^2} \int_\Gamma |\nabla_\Gamma v|^2 \, do \quad \forall v \in H^1_V(\Gamma),$$

see Lemma 4.2.2 for a proof. Thus the bilinear form on the left hand side of (4.31) is coercive and, given $w \in W^{1,p}_V(\Gamma) \subset L^2_V(\Gamma)$, existence and uniqueness for (4.31) follows by the Lax-Milgram theorem. Finally, by elliptic regularity we obtain $u \in W^{3,p}(\Gamma)$. □

We can now prove the equivalence of the two formulations.

Proposition 4.5.2. *The pair (w, u) solves Problem 4.5.4 if and only if u is the unique solution of Problem 4.5.1 and $w = -\Delta_\Gamma u - (2/R^2)u$.*

Proof. Suppose (w, u) solves Problem 4.5.4. By the regularity result we have $u \in W^{3,p}_V(\Gamma) \subset W^2_V(\Gamma)$ and $w = -\Delta_\Gamma u - (2/R^2)u$ in the sense of weak derivatives. We then use equations (4.30) and (4.31) with test functions $v \in H^2_V(\Gamma)$,

$$\begin{aligned}\int_\Gamma \kappa \left(\Delta_\Gamma u \Delta_\Gamma v - \frac{2}{R^2} \nabla_\Gamma u \cdot \nabla_\Gamma v \right) + \sigma \left(\nabla_\Gamma u \cdot \nabla_\Gamma v - \frac{2}{R^2} uv \right) &= \int_\Gamma w \left(-\kappa \Delta_\Gamma v + \sigma v \right), \\ &= \langle \tilde{\delta}_X, v \rangle.\end{aligned}$$

This is equivalent to u solving Problem 4.5.1. The reverse implication then follows by uniqueness for each problem. □

We now relate this problem with integral constraints to Problem 4.5.3 which we discretise to form the numerical method.

Proposition 4.5.3. *Problem 4.5.3 admits a unique solution, moreover the solution is the solution to Problem 4.5.4.*

Proof. We first show (w, u), the solution to Problem 4.5.4, is a solution to Problem 4.5.3. Let $v \in W^{1,q}(\Gamma)$ and $P : L^2(\Gamma) \to L^2_\sigma(\Gamma)$ be the canonical projection (note that this is simply the identity mapping if $\sigma > 0$),

$$\begin{aligned}\int_\Gamma \kappa \nabla_\Gamma w \cdot \nabla_\Gamma v + \sigma w v \, do + \chi_\sigma (w, 1)_{L^2(\Gamma)} (v, 1)_{L^2(\Gamma)} &= \int_\Gamma \kappa \nabla_\Gamma w \cdot \nabla_\Gamma P v + \sigma w P v \, do, \\ &= \langle \tilde{\delta}_X, P v \rangle, \\ &= \langle \tilde{\delta}_X, v \rangle.\end{aligned}$$

Now let $v \in H^1(\Gamma)$ and express this as $v = h + \alpha_0 + \alpha_1\nu_1 + \alpha_2\nu_2 + \alpha_3\nu_3$ with $h \in H^1_V(\Gamma)$,

$$
\begin{aligned}
\int_\Gamma \nabla_\Gamma u \cdot \nabla_\Gamma v - \frac{2}{R^2} uv \, do + \tau \sum_{i=1}^{4} (u, g_i)_{L^2(\Gamma)} (v, g_i)_{L^2(\Gamma)}, &= \int_\Gamma \nabla_\Gamma u \cdot \nabla_\Gamma h - \frac{2}{R^2} uh \, do, \\
&= \int_\Gamma wh \, do, \\
&= \int_\Gamma wv \, do.
\end{aligned}
$$

Thus (w, u) as stated is a solution to Problem 4.5.3. For uniqueness, suppose w_1, w_2 satisfy the first equation of Problem 4.5.3, testing with $v \in H^2_\sigma(\Gamma)$ produces

$$
0 = \int_\Gamma P(w_1 - w_2) \left(-\kappa \Delta_\Gamma v + \sigma v\right).
$$

As $-\Delta_\Gamma + \sigma I$ maps $H^2_\sigma(\Gamma)$ onto $L^2_\sigma(\Gamma)$ it follows $P(w_1 - w_2) = 0$. If $\sigma > 0$ then $P = I$ and we are done, if $\sigma = 0$ testing with $v = 1$ then shows $(w_1 - w_2, 1)_{L^2(\Gamma)} = 0$ thus we have uniqueness for the first equation. For the second equation note that the inner product

$$
(u, v) \mapsto \int_\Gamma \nabla_\Gamma u \cdot \nabla_\Gamma v - \frac{2}{R^2} uv \, do + \lambda \sum_{i=1}^{4} (u, g_i)_{L^2(\Gamma)} (v, g_i)_{L^2(\Gamma)}
$$

is coercive over $H^1(\Gamma)$ for any $\lambda > 1/(2\pi R^4)$. To see this, note that for any $u \in H^1(\Gamma)$ we may write

$$
u = u_V + \sum_{i=1}^{4} \frac{(u, g_i)_{L^2(\Gamma)}}{(g_i, g_i)_{L^2(\Gamma)}} g_i.
$$

with $u_V \in H^1_V(\Gamma)$. It follows

$$
\begin{aligned}
(u, u) \mapsto & \int_\Gamma |\nabla_\Gamma u_V|^2 - \frac{2}{R^2} u_V^2 \, do - \int_\Gamma \frac{2}{R^2} \frac{(u, 1)^2_{L^2(\Gamma)}}{(1, 1)^2_{L^2(\Gamma)}} \, do + \lambda \sum_{i=1}^{4} \frac{(u, g_i)^2_{L^2(\Gamma)}}{(g_i, g_i)_{L^2(\Omega)}} \\
& \geq C \|u_V\|^2_{1,2} + \left(\lambda - \frac{1}{2\pi R^2}\right) (u, 1)_{L^2(\Gamma)} + \lambda \sum_{i=2}^{4} \frac{(u, g_i)^2_{L^2(\Gamma)}}{(g_i, g_i)_{L^2(\Gamma)}} \\
& \geq C \|u\|^2_{H^1(\Gamma)}
\end{aligned}
$$

with the final line holding if $\lambda - 1/(2\pi R^4) > 0$. Given coercivity, uniqueness is then a consequence of the Lax-Milgram theorem. $\square$

4.6 Numerical studies

4.6.1 Surface finite element methods

In this section we present some preliminary illustrative numerical results concerning problems formulated in Section 4.4 concerning the Willmore functional. Our numerical studies are performed using surface finite elements, [27]. The underlying partial differential equations are of fourth order. In order to avoid the use of H^2 conforming surface finite elements we use second order splitting to obtain two coupled second order surface equations which can be approximated by continuous piecewise linear surface finite elements on triangulated surfaces.

We now assume that the undeformed surface Γ is approximated by a polyhedral hypersurface

$$\Gamma_h = \bigcup_{T \in \mathcal{T}_h} T,$$

where $\mathcal{T}_h$ denotes the set of two-dimensional simplices in $\mathbb{R}^3$ which are supposed to form an admissible triangulation. Recall that our problems are posed on either a sphere or a Clifford torus. The approach is also applicable to similar PDEs on other closed surfaces. We assume that Γ_h is contained in a strip $\mathcal{N}_\delta$ of width $\delta > 0$ on which the decomposition

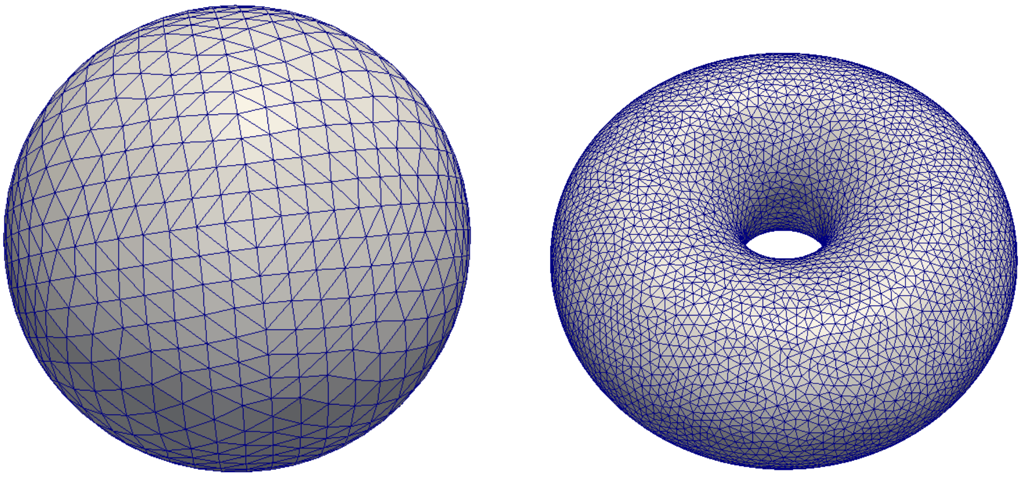
$$x = p + d(x)\nu(p), \quad p \in \Gamma$$

is unique for all $x \in \mathcal{N}_\delta$. Here, $d(x)$ denotes the oriented distance function to Γ, see Section 2.2 in [18]. This defines a map $x \mapsto p(x)$ from $\mathcal{N}_\delta$ onto Γ. We here assume that the restriction $p_{|\Gamma_h}$ of this map onto the polyhedral hypersurface Γ_h is a bijective map between Γ_h and Γ. In addition, the vertices of the simplices $T \in \mathcal{T}_h$ are supposed to sit on Γ. The generation of these triangulations for the sphere and torus is rather standard, see for example [27]. In Figure 4.1 we show typical triangulations.

The piecewise linear Lagrange finite element space on Γ_h is

$$\mathcal{S}_h := \{\chi \in C(\Gamma_h) \mid \chi_T \in \mathbb{P}_1(T) \; \forall T \in \mathcal{T}_h\},$$

where $\mathbb{P}_1(T)$ denotes the set of polynomials of degree 1 on T. The Lagrange basis functions φ_i of this space are uniquely determined by their values at the so-called Lagrange nodes q_j, that is $\varphi_i(q_j) = \delta_{ij}$. The associated Lagrange interpolations for



(a) Example triangulation for a sphere (b) Example triangulation for a torus

Figure 4.1: Example triangulations of surfaces.

a continuous function f on Γ_h are defined by

$$I_h^r f := \sum_i f(q_i)\varphi_i.$$

For a function defined on Γ_h, $v_h : \Gamma_h \to \mathbb{R}$ we use the bijection $p_{|\Gamma_h}$ to define the standard lift operator, that is we define the function $v_h^l : \Gamma \to \mathbb{R}$ by

$$v_h^l(x) := v_h(p_{|\Gamma_h}^{-1} x).$$

Similarly for a function $v : \Gamma \to \mathbb{R}$ we define the downwards lift by $v^{-l} : \Gamma_h \to \mathbb{R}$ such that

$$v^{-l}(x_h) := v(p_{|\Gamma_h}(x_h)).$$

4.6.2 Discretisation of Problem 4.5.3

We discretise the system using P^1 finite elements, for this we require the following notation.

Definition 4.6.1. *For $u_h, v_h \in \mathcal{S}_h$, define the following functionals*

$$
\begin{aligned}
s_h(u_h, v_h) &:= \int_{\Gamma_h} \nabla_{\Gamma_h} u_h \cdot \nabla_{\Gamma_h} u_h \, do_h, \\
m_h(u_h, v_h) &:= \int_{\Gamma_h} u_h v_h \, do_h, \\
b_h(u_h, v_h) &:= \int_{\Gamma_h} u_h \, do_h \int_{\Gamma_h} v_h \, do_h + \sum_{i=1}^{3} \int_{\Gamma_h} u_h \nu_i^{-l} \, do_h \int_{\Gamma_h} u_h \nu_i^{-l} \, do_h, \\
\langle \tilde{\delta}_X^h, v_h \rangle &:= \sum_{k=1}^{N} \beta_k v_h^l(X_k) - \frac{1}{4\pi R^2} \int_{\Gamma_h} v_h \, do_h - \frac{3}{4\pi R^2} \sum_{r=1}^{3} \nu_r(X_k) \int_{\Gamma_h} v_h \nu_r^{-l} \, do_h.
\end{aligned}
$$

Note that the functions $1, \nu_1, \nu_2, \nu_3$ appearing in $b_h(\cdot, \cdot)$ above are precisely the functions g_1, g_2, g_3, g_4 on a sphere. The following geometric perturbation errors are an immediate consequence of [27, Lemma 4.7].

Lemma 4.6.1. *There exists $C > 0$ such that for all $h > 0$ and all $u_h, v_h \in \mathcal{S}_h$*

$$
\begin{aligned}
\left| \int_\Gamma \nabla_\Gamma u_h^l \cdot \nabla_\Gamma v_h^l \, do - s_h(u_h, v_h) \right| &\le Ch^2 \|u_h^l\|_{H^1(\Gamma)} \|v_h^l\|_{H^1(\Gamma)}, \\
\left| \int_\Gamma u_h^l v_h^l \, do - m_h(u_h, v_h) \right| &\le Ch^2 \|u_h^l\|_{L^2(\Gamma)} \|v_h^l\|_{L^2(\Gamma)}, \\
\left| \int_\Gamma u_h^l \, do \int_\Gamma v_h^l \, do + \sum_{i=1}^{3} \int_\Gamma u_h^l \nu_i \, do \int_\Gamma v_h^l \nu_i \, do - b_h(u_h, v_h) \right| &\le Ch^2 \|u_h^l\|_{L^2(\Gamma)} \|v_h^l\|_{L^2(\Gamma)}.
\end{aligned}
$$

The resulting discretised system then reads as follows.

Problem 4.6.1. *Find $u_h, w_h \in \mathcal{S}_h$ such that for all $v_h \in \mathcal{S}_h$*

$$
(\kappa s_h + \sigma m_h)(w_h, v_h) + \chi_\sigma m_h(w_h, 1) m_h(v_h, 1) = \langle \tilde{\delta}_X^h, v_h \rangle, \tag{4.32}
$$

$$
(s_h - \frac{2}{R^2} m_h + \tau b_h)(u_h, v_h) = m_h(w_h, v_h). \tag{4.33}
$$

We conclude this section by showing that Problem 4.6.1, the discretised problem we solve for the finite element approximation, is well posed. We will then prove convergence in later sections.

Lemma 4.6.2. *Problem 4.6.1 admits a unique solution for h sufficiently small.*

Proof. Beginning with (4.32), we will prove coercivity for the discrete bilinear functional,

$$
(u_h, v_h) \mapsto (\kappa s_h + \sigma m_h)(w_h, v_h) + \chi_\sigma m_h(w_h, 1) m_h(v_h, 1),
$$

this implies uniqueness for the first equation and hence existence as the problem is finite dimensional. Using that the full bilinear functional is coercive and Lemma 4.6.1, there exists $C_1, C_2 > 0$ such that, for any $v_h \in V_h$

$$
\begin{aligned}
C_1 \|v_h^l\|_{H^1(\Gamma)}^2 &\leq \int_\Gamma \kappa |\nabla_\Gamma v_h^l|^2 + \sigma (v_h^l)^2 \, do + \chi_\sigma \left(\int_\Gamma v_h^l \, do \right)^2 \\
&\leq \kappa s_h(v_h, v_h) + \sigma m_h(v_h, v_h) + \chi_\sigma m_h(v_h, 1)^2 + C_2 h^2 \|v_h^l\|_{H^1(\Gamma)}^2.
\end{aligned}
$$

Thus $\kappa s_h + \sigma m_h + c_h$ is coercive over V_h for any $0 < h < \sqrt{C_1/2C_2}$. Hence (4.32) admits a unique solution for sufficiently small h. An identical argument may be applied for (4.33). Thus the pair (w_h, u_h) is unique. $\square$

We will now prove error estimates for this method. We will begin with the equation for w in Problem 4.5.3, note that the well posedness of this equation does not rely on the surface Γ being spherical. As such we will present an error estimate for this equation on a more general surface.

4.6.3 Surface finite element method for a Poisson equation with singular data

The variational formulation, Problem 4.5.3 has less regularity than the more standard setting in which we have an L^2 right hand side. We are thus not able to obtain the optimal convergence rates of $O(h)$ and $O(h^2)$ in the H^1 and L^2 norms respectively for $w_h^l - w$. We instead recover $O(h)$ convergence in the L^2 norm for w_h^l, as seen for a similar problem over a flat domain in [14, 71] and Chapter 2 of this thesis. This is sufficient to produce almost optimal convergence rates for $u_h^l - u$.

In this section we will consider $\Gamma \subset \mathbb{R}^3$ to be a two dimensional surface which is smooth, compact and connected. The principal application here will be to a sphere but the convergence result shown is more general. Similarly we will generalise the functional on the right hand side to any $\mu \in C^0(\Gamma)^*$. For clarity the general smooth problem and the finite element approximation are stated below.

Problem 4.6.2. *Suppose $\Gamma \subset \mathbb{R}^3$ is a two dimensional surface which is smooth, compact and connected. Let $\mu \in C^0(\Gamma)^*$ and fix $p \in (1,2)$ and $q \in (2,\infty)$ such that $1/p + 1/q = 1$. Find $\zeta \in W^{1,p}_\sigma(\Gamma)$ such that*

$$
\int_\Gamma \kappa \nabla_\Gamma \zeta \cdot \nabla_\Gamma v + \sigma \zeta v \, do = \langle \mu, v \rangle \qquad \forall v \in W^{1,q}_\sigma(\Gamma),
$$

where we additionally assume $\langle \mu, 1 \rangle = 0$ if $\sigma = 0$.

The well posedness of this problem can be proven by the argument used for (4.30) in Proposition 4.5.1. The argument can also be used to produce the bound

$$\|\zeta\|_{L^2(\Gamma)} \leq C\|\mu\|_{C^0(\Gamma)^*}. \tag{4.34}$$

We now state the discretised problem.

Problem 4.6.3. *Let $\mu^h \in (V_h)^*$, with $\langle \mu^h, 1\rangle = 0$ if $\sigma = 0$, find $\zeta_h \in V_h$ such that*

$$\kappa s_h(\zeta_h, v_h) + \sigma m_h(\zeta_h, v_h) + \chi_\sigma(\zeta_h, 1)_{L^2(\Gamma_h)}(v_h, 1)_{L^2(\Gamma_h)} = \langle \mu^h, v_h\rangle \qquad \forall v_h \in V_h,$$

where $\chi_\sigma = 1$ if $\sigma = 0$ and $\chi_\sigma = 0$ otherwise.

The well posedness of this problem follows from the coercivity result shown in Lemma 4.6.2, which holds on the more general surface used here. We now prove convergence of this finite element method. The proof uses a similar technique to [14], which proves the analogous result for a finite element method over a flat domain.

Theorem 4.6.1. *Let ζ_h denote the solution to Problem 4.6.3 and ζ the solution to Problem 4.6.2. Suppose there exists $C_1 > 0$, independent of h, such that*

$$|\langle \mu, v_h^l\rangle - \langle \mu^h, v_h\rangle| \leq C_1 h\|\mu\|_{C^0(\Gamma)^*}\|v_h^l\|_{H^1(\Gamma)}.$$

Then there exists $C(\Gamma) > 0$ such that, for sufficiently small h,

$$\|\zeta_h^l - \zeta\|_{L^2(\Gamma)} \leq Ch\|\mu\|_{C^0(\Gamma)^*}.$$

Proof. Let $f \in L^2_\sigma(\Gamma)$ and $\psi \in H^2_\sigma(\Gamma)$ be such that

$$\int_\Gamma \kappa\nabla_\Gamma\psi \cdot \nabla_\Gamma v + \sigma\psi v \, do = \int_\Gamma fv \, do \quad \text{for all } v \in H^1_\sigma(\Gamma). \tag{4.35}$$

That $\psi \in H^2(\Gamma)$ is a result of elliptic regularity (see [27, Theorem 3.3]), from which we also obtain the estimate $\|\psi\|_{H^2(\Gamma)} \leq C\|f\|_{L^2(\Gamma)}$ for some constant $C > 0$ which is independent of f, ψ. Construct $f_h \in L^2(\Gamma_h)$ by

$$f_h := \hat{f} - \chi_\sigma\left(\frac{1}{|\Gamma_h|}\int_{\Gamma_h}\hat{f}\right)1,$$

with $\hat{f} : \Gamma_h \to \mathbb{R}^3$ defined by $\hat{f}(\hat{x}) := f(p^{-1}_{|\Gamma_h}(\hat{x}))$, it follows

$$\|f_h^l - f\|_{L^2(\Gamma)} \leq Ch^2\|f\|_{L^2(\Gamma)}.$$

Let $\psi_h \in V_h$ be such that

$$\kappa s_h(\psi_h, v_h) + \sigma m_h(\psi_h, v_h) = m_h(f_h, v_h) \qquad \forall v_h \in V_h, \tag{4.36}$$

with uniqueness ensured when $\sigma = 0$ by choosing $\int_{\Gamma_h} \psi_h = 0$. Letting $I_h\psi$ denote the P^1 interpolant of ψ, we will now derive an L^∞ estimate for $\psi_h^l - \psi$.

$$\begin{aligned}
\|\psi_h^l - \psi\|_{L^\infty(\Gamma)} &\leq \|\psi - (I_h\psi)^l\|_{L^\infty(\Gamma)} + \|\psi_h^l - (I_h\psi)^l\|_{L^\infty(\Gamma)} \\
&= \|\hat{\psi} - (I_h\psi)\|_{L^\infty(\Gamma_h)} + \|\psi_h - (I_h\psi)\|_{L^\infty(\Gamma_h)} \\
&\leq Ch \max_{T \in \mathcal{T}_h} \|\hat{\psi}\|_{H^2(T)} + Ch^{-1}\|\psi_h - I_h\psi\|_{L^2(\Gamma_h)} \\
&\leq Ch\|\psi\|_{H^2(\Gamma)} + Ch\|f\|_{L^2(\Gamma)}
\end{aligned}$$

The bounds used on the third line are produced using element-wise estimates given in [15], Theorem 3.1.5 and Theorem 3.2.6 respectively. To proceed to the final line the terms are bounded using Lemma 4.2, Lemma 4.3 and Theorem 4.9 in [27]. We now produce the bound for $\zeta_h^l - \zeta$,

$$\begin{aligned}
\left|\int_\Gamma (\zeta - \zeta_h^l) f\right| &= \left|\int_\Gamma \kappa \nabla_\Gamma \psi \cdot \nabla_\Gamma \zeta + \sigma\psi\zeta \, do - \kappa s_h(\psi_h, \zeta_h) - \sigma m_h(\psi_h, \zeta_h)\right| \\
&\quad + \left|\int_{\Gamma_h} \zeta_h f_h - \int_\Gamma \zeta_h^l f_h^l\right| + \left|\int_\Gamma \zeta_h^l (f_h^l - f)\right| \\
&\leq |\langle \mu, \psi\rangle - \langle \mu^h, \psi_h\rangle| + \left|\int_{\Gamma_h} \zeta_h f_h - \int_\Gamma \zeta_h^l f_h^l\right| + \left|\int_\Gamma \zeta_h^l (f_h^l - f)\right| \\
&\leq \|\mu\|_{C^0(\Gamma)^*} \left(\|\psi_h^l - \psi\|_{L^\infty(\Gamma)} + Ch\|\psi_h^l\|_{H^1(\Gamma)}\right) + Ch^2\|f\|_{L^2(\Gamma)}\|\zeta_h^l\|_{L^2(\Gamma)}, \\
&\leq Ch\|\mu\|_{C^0(\Gamma)^*}\|f\|_{L^2(\Gamma)} + Ch^2\|f\|_{L^2(\Gamma)}\|\zeta_h^l\|_{L^2(\Gamma)}.
\end{aligned} \tag{4.37}$$

The second line follows by the a priori bound $\|\psi_h^l\|_{H^1(\Gamma)} \leq C\|f\|_{L^2(\Gamma)}$ and Lemma 4.7 in [27]. Now taking the supremum over $f \in L^2(\Gamma)$ with $\|f\|_{L^2(\Gamma)} = 1$, using the triangle inequality and the bound in (4.34) produces

$$\|\zeta - \zeta_h^l\|_{L^2(\Gamma)} \leq C(h + h^2)\|\mu\|_{C^0(\Gamma)^*} + Ch^2\|\zeta - \zeta_h^l\|_{L^2(\Gamma)}.$$

We can then complete the proof by taking h sufficiently small such that the second term on the right hand side can be absorbed into the left hand side. $\square$

4.6.4 Error analysis for Problem 4.6.1

We now return to assuming Γ is a sphere for the analysis of the full system. Notice however, the restriction to a spherical surface does not reflect a limitation in the finite element method so much as a lack of well posedness for the underlying variational problem.

Theorem 4.6.2. *Let (w_h, u_h) denote the solution to Problem 4.6.1 and (w, u) the solution to Problem 4.5.3. There exists $C > 0$ such that, for sufficiently small h,*

$$\begin{aligned} \|w_h^l - w\|_{L^2(\Gamma)} + \|u_h^l - u\|_{H^1(\Gamma)} &\leq Ch\|\tilde{\delta}_X\|_{C^0(\Gamma)^*}, \\ \|u_h^l - u\|_{L^2(\Gamma)} &\leq Ch^2|\log(h)|\|\tilde{\delta}_X\|_{C^0(\Gamma)^*}. \end{aligned}$$

Proof. The $\|w_h^l - w\|_{L^2(\Gamma)}$ estimate is shown in Theorem 4.6.1, we need only check the assumption

$$|\langle \mu, v_h^l \rangle - \langle \mu^h, v_h \rangle| \leq Ch\|\mu\|_{C^0(\Gamma)^*}\|v_h\|_{H^1(\Gamma)}.$$

In this context $\mu = \tilde{\delta}_X$ and $\mu^h = \tilde{\delta}_X^h$, thus

$$\begin{aligned} \left|\langle \tilde{\delta}_X, v_h^l \rangle - \langle \tilde{\delta}_X^h, v_h \rangle\right| &\leq \frac{N}{4\pi R^2}\left|\int_\Gamma v_h^l - \int_{\Gamma_h} v_h\right| + \frac{3}{4\pi R^2}\sum_{k=1}^N\sum_{i=1}^3 |\nu_i(X_k)|\left|\int_\Gamma v_h^l \nu_i - \int_{\Gamma_h} v_h \hat{\nu}_i\right|, \\ &\leq Ch^2\|v_h^l\|_{L^2(\Gamma)}. \end{aligned}$$

Taking $h < \|\tilde{\delta}_X\|_{C^0(\Gamma)^*}$ (note that the $\tilde{\delta}_X = 0$ is trivial), this is a sufficient bound to apply Theorem 4.6.1 from which the estimate on $\|w_h^l - w\|_{L^2(\Gamma)}$ is immediate. The H^1 estimate for $u_h^l - u$ now follows, using the second equation of the system (4.33), we argue as in [27, Theorem 4.9]. For brevity we introduce the following notation

$$\begin{aligned} m(u, v) &:= \int_\Gamma uv \, do, \\ m_h(u_h, v_h) &:= \int_{\Gamma_h} u_h v_h \, do_h, \\ A(u, v) &:= \int_\Gamma \nabla_\Gamma u \cdot \nabla_\Gamma v - \frac{2}{R^2} uv \, do + \tau\sum_{i=1}^4 (u, g_i)_{L^2(\Gamma)}(v, g_i)_{L^2(\Gamma)}, \\ A_h(u_h, v_h) &:= \int_{\Gamma_h} \nabla_{\Gamma_h} u_h \cdot \nabla_{\Gamma_h} v_h - \frac{2}{R^2} u_h v_h \, do + \tau\sum_{i=1}^4 (u_h, g_i \circ p)_{L^2(\Gamma_h)}(v_h, g_i \circ p)_{L^2(\Gamma_h)}. \end{aligned}$$

A coercivity result holds for $A_h(\cdot, \cdot)$, using the argument in Lemma 4.6.2. In addition a geometric perturbation estimate holds by [27, Lemma 4.7],

$$|A(u_h^l, v_h^l) - A_h(u_h, v_h)| \leq Ch^2 \|u_h^l\|_{H^1(\Gamma)} \|v_h^l\|_{H^1(\Gamma)}.$$

Now let $\phi_h \in V_h$ with corresponding lift ϕ_h^l,

$$\begin{aligned}
C_1\|u_h^l - \phi_h^l\|_{H^1(\Gamma)}^2 &\leq A_h(u_h - \phi_h, u_h - \phi_h), \\
&= A(u - \phi_h^l, u_h^l - \phi_h^l) + A(\phi_h^l, u_h^l - \phi_h^l) - A_h(\phi_h, u_h - \phi_h) \\
&\quad - \left(m(w, u_h^l - \phi_h^l) - m(w_h^l, u_h^l - \phi_h^l)\right) - \left(m(w_h^l, u_h^l - \phi_h^l) - m_h(w_h, u_h - \phi_h)\right), \\
&\leq C\|u - \phi_h^l\|_{H^1(\Gamma)} \|u_h^l - \phi_h^l\|_{H^1(\Gamma)} + Ch^2 \|\phi_h^l\|_{H^1(\Gamma)} \|u_h^l - \phi_h^l\|_{H^1(\Gamma)} \\
&\quad + \|w - w_h^l\|_{L^2(\Gamma)} \|u_h^l - \phi_h^l\|_{L^2(\Gamma)} + Ch^2 \|w_h^l\|_{L^2(\Gamma)} \|u_h^l - \phi_h^l\|_{L^2(\Gamma)}.
\end{aligned}$$

Dividing out the factor of $\|u_h^l - \phi_h^l\|_{H^1(\Gamma)}$ produces the inequality

$$\|u_h^l - \phi_h^l\|_{H^1(\Gamma)} \leq C\left(\|u - \phi_h^l\|_{H^1(\Gamma)} + h^2\|\phi_h^l\|_{H^1(\Gamma)} + \|w - w_h^l\|_{L^2(\Gamma)} + h^2\|w_h^l\|_{L^2(\Gamma)}\right).$$

Now set $\phi_h = I_h u$, the discrete interpolant of u, then $\|u - (I_h u)^l\|_{H^1(\Gamma)} \leq Ch\|u\|_{H^2(\Gamma)}$ and $\|(I_h u)^l\|_{H^1(\Gamma)} \leq C\|u\|_{H^2(\Gamma)}$. Using the convergence result for $w - w_h^l$ we thus obtain the bound

$$\|u_h^l - (I_h u)^l\|_{H^1(\Gamma)} \leq Ch\|u\|_{H^2(\Gamma)}.$$

From this the required bound follows

$$\|u_h^l - u\|_{H^1(\Gamma)} \leq \|u_h^l - (I_h u)^l\|_{H^1(\Gamma)} + \|u - (I_h u)^l\|_{H^1(\Gamma)} \leq Ch\|u\|_{H^2(\Gamma)} \leq Ch\|\tilde{\delta}_X\|_{C^0(\Gamma)^*}.$$

The bound used for the final equality is immediate from the variational formulation, Problem 4.5.1. The L^2 bound will be produced by the Aubin-Nitsche trick, we first estimate the quantity

$$\|w_h^l - w\|_* := \sup\left\{|m(w_h^l - w, f)| \mid f \in W^{1,q}(\Gamma) \text{ and } \|f\|_{W^{1,q}(\Gamma)} = 1\right\},$$

recall q is chosen such that $q > 2$. To estimate this quantity, take f, f_h, ψ, ψ_h as constructed in (4.35) and (4.36) except now assume additionally that $f \in W^{1,q}(\Gamma)$ hence by elliptic regularity $\psi \in W^{3,q}(\Gamma)$. With this additional regularity one can improve the bound obtained in (4.37). Using [21, Corollary 4.6] and [15, Theorem

3.1.6] produces, for any $p \in (2,\infty)$,

$$
\begin{aligned}
\|\psi - \psi_h^l\|_{L^\infty(\Gamma)} &\leq Ch|log(h)| \inf_{\chi \in V_h} \|\nabla_\Gamma(\psi - \chi^l)\|_{L^\infty(\Gamma)} + Ch^2|\log(h)|\|\psi\|_{H^3(\Gamma)}, \\
&\leq Ch^2|\log(h)|(\|\psi\|_{W^{2,\infty}(\Gamma)} + \|\psi\|_{H^3(\Gamma)}), \\
&\leq Ch^2|\log(h)|\|f\|_{W^{1,q}(\Gamma)}.
\end{aligned}
$$

Note that the bound used from [21] is proven explicitly only for the case $\sigma = 0$. It may be extended to the $\sigma > 0$ case using the argument outlined in the final section of that paper. For this we need an appropriate analogue of [21, Lemma 2.2]. Returning to (4.37) with this improved bound produces

$$
\|w_h^l - w\|_* \leq Ch^2|\log(h)|\|\tilde{\delta}_X\|_{C^0(\Gamma)^*}.
$$

We now perform the Aubin-Nitsche trick to produce the bound. Let $\varphi \in H^2(\Gamma)$ such that

$$
m(u_h^l - u, v) = A(\varphi, v) \quad \forall v \in H^1(\Gamma),
$$

note we have the regularity estimate $\|\varphi\|_{H^2(\Gamma)} \leq C\|u_h^l - u\|_{L^2(\Gamma)}$. Let $v_h \in V_h$, it follows

$$
\begin{aligned}
m(u_h^l - u, u_h^l - u) &= A(u_h^l - u, \varphi - v_h^l) + A(u_h^l - u, v_h^l), \\
&= A(u_h^l - u, \varphi - v_h^l) + m(w_h^l - w, v_h^l) + m_h(w_h, v_h) - m(w_h^l, v_h^l) \\
&\quad + A(u_h^l, v_h^l) - A_h(u_h, v_h).
\end{aligned}
$$

Setting $v_h = I_h\varphi$ then produces

$$
\begin{aligned}
&\|u_h^l - u\|_{L^2(\Gamma)}^2 \\
&\quad \leq Ch^2\|u_h^l - u\|_{L^2(\Gamma)} \left(\|u\|_{H^2(\Gamma)} + |\log(h)|\|\tilde{\delta}_X\|_{C^0(\Gamma)^*} + \|w_h^l\|_{L^2(\Gamma)} + \|u_h^l\|_{H^1(\Gamma)} \right), \\
&\quad \leq Ch^2|\log(h)|\|u_h^l - u\|_{L^2(\Gamma)},
\end{aligned}
$$

from which the required bound is immediate. □

4.6.5 Numerical convergence testing

To test the numerical method we first construct the exact solution (w, u) to Problem 4.5.3. In this section, for simplicity of constructing the exact solution, we will take $R = 1$, $\sigma = 0$, $N = 1$, $\beta_1 = 1$ and $X = (0, 0, 1)$. Using [49] we see, using the standard spherical coordinates $x(\theta, \varphi)$,

$$-\Delta_\Gamma \left[-\frac{1}{4\pi} \log \left(\frac{1 - \cos(\theta)}{2} \right) - \frac{1}{4\pi} \right] = \delta_X - \frac{1}{4\pi}.$$

Note that we have fixed the additive constant so that this fundamental solution has zero integral. It follows, since $-\Delta_\Gamma \nu_i = 2\nu_i$ for each $i = 1, 2, 3$,

$$w(x(\theta, \varphi)) = -\frac{1}{4\pi} \log \left(\frac{1 - \cos(\theta)}{2} \right) - \frac{1}{4\pi} - \frac{3}{8\pi} \cos(\theta).$$

As w is independent of φ we look for a solution u that is likewise, hence we look to solve an ordinary differential equation for $U(\theta) := u(x(\theta, \varphi))$,

$$-\frac{1}{\sin(\theta)} \frac{d}{d\theta} \left(\sin(\theta) \frac{dU}{d\theta} \right) - 2U = w(x(\theta, \varphi)). \tag{4.38}$$

A particular solution is given by

$$F(\theta) = \frac{1}{8\pi} \left[(1 - \cos(\theta)) \log(1 - cos(\theta)) + \frac{1}{2} - \log(2) \right].$$

Notice, defining $f(x(\theta, \phi)) := F(\theta)$, it holds

$$\int_\Gamma f = \int_\Gamma f\nu_1 = \int_\Gamma f\nu_2 = 0.$$

Furthermore, $\nu_3(x(\theta, \phi)) = cos(\theta)$ which satisfies the homogeneous version of (4.38), thus to find U we project out the $cos(\theta)$ component of F, producing

$$u(x(\theta, \phi)) = \frac{1}{8\pi} \left[(1 - \cos(\theta)) \log(1 - cos(\theta)) + \left(\frac{1}{6} + \log(2) \right) \cos(\theta) + \frac{1}{2} - \log(2) \right].$$

To carry out the error testing we begin with a coarse mesh consisting of six vertices

$$\{(\pm 1, 0, 0), (0, \pm 1, 0), (0, 0, \pm 1)\}$$

with the elements being the faces of the regular octahedron these vertices form. At each refinement step we use the refine and project method detailed in [27, Figure 4.3]. Precisely, given a mesh, we form the next refinement by adding nodes at the midpoint of each edge and projecting them onto the sphere. Refining in this manner ensures that h, the maximum diameter of an element, is halved each time. We thus compute the experimental order of convergence in the norm $\|\cdot\|_Y$ between successive refinements via the formula

$$EOC(u, Y, h_n) = \log\left(\frac{E_Y(h_{n-1})}{E_Y(h_n)}\right) / \log(2),$$

where $n \geq 1$ denotes the number of refinements, h_n the maximum diameter of an element after n refinements and $E_Y(h_n)$ denotes the error of the approximation in the Y norm, $\|u - u^l_{h_n}\|_Y$. The finite element method was implemented using the DUNE-FEM module [19] and the convergence results are tabulated below.

The data for the convergence of u^l_h is shown in Table 4.1. These results confirm the optimality of the theoretical results in Theorem 4.6.2, showing an experimental order of convergence of 1 for the $H^1(\Gamma)$ norm, which agrees with the bound proven. For the $L^2(\Gamma)$ norm the experimental orders of convergence are consistent with an error which decays as $h^2|\log(h)|$. The data for the convergence of w^l_h is shown in Table 4.2. These results also agree with Theorem 4.6.2 showing the EOC for the $L^2(\Gamma)$ error is 1. There is no $H^1(\Gamma)$ convergence here as $w \notin H^1(\Gamma)$.

h_n	$E_{L^2(\Gamma)}(h_n)$	EOC	$E_{H^1(\Gamma)}(h_n)$	EOC
1.41421	1.44401×10^{-2}	-	3.37676×10^{-2}	-
7.07106×10^{-1}	1.25032×10^{-2}	0.207787	3.65949×10^{-2}	-0.116005
3.53553×10^{-1}	5.63549×10^{-3}	1.14968	2.24354×10^{-2}	0.705865
1.76776×10^{-1}	1.92398×10^{-3}	1.55045	1.17367×10^{-2}	0.93475
8.83883×10^{-2}	5.76858×10^{-4}	1.73781	5.9068×10^{-3}	0.990579
4.41941×10^{-2}	1.63771×10^{-4}	1.81654	2.95445×10^{-3}	0.999488
2.20970×10^{-2}	4.53712×10^{-5}	1.85183	1.47689×10^{-3}	1.00033
1.10485×10^{-2}	1.24076×10^{-5}	1.87056	7.38341×10^{-4}	1.0002
5.52427×10^{-3}	3.36457×10^{-6}	1.88273	3.69149×10^{-4}	1.00009
2.76213×10^{-3}	9.06562×10^{-7}	1.89194	1.84570×10^{-4}	1.00003

Table 4.1: Errors and Experimental orders of convergence for $u^l_h - u$.

h_n	$E_{L^2(\Gamma)}(h_n)$	EOC
1.41421	1.43529×10^{-1}	-
7.07106×10^{-1}	6.16088×10^{-2}	1.22013
3.53553×10^{-1}	2.63191×10^{-2}	1.22702
1.76776×10^{-1}	1.29302×10^{-2}	1.02536
8.83883×10^{-2}	6.61726×10^{-3}	0.966444
4.41941×10^{-2}	3.36201×10^{-3}	0.97691
2.20970×10^{-2}	1.69309×10^{-3}	0.989666
1.10485×10^{-2}	8.48850×10^{-4}	0.996076
5.52427×10^{-3}	4.24826×10^{-4}	0.998638
2.76213×10^{-3}	2.12479×10^{-4}	0.999553

Table 4.2: Errors and Experimental orders of convergence for $w_h^l - w$.

4.6.6 Point constraints for a Clifford torus

We also solve Problem 4.4.4 numerically, enforcing the constraint $u \in U = (H^2_{X,0} \cap Ker(a))^\perp$ via a penalty method. As in the previous algorithm we will express the condition $u \in U$ via $L^2(\Gamma)$-orthogonality. That is, for each basis function of $H^2_{X,0} \cap Ker(a)$, f_i, set

$$g_i := (\Delta_\Gamma^2 - \Delta_\Gamma + 1) f_i \in C^\infty(\Gamma).$$

We can then characterise U in terms of $L^2(\Gamma)$-orthogonality with the g_i, for $1 \leq i \leq L := dim(H^2_{X,0} \cap Ker(a))$

$$U = \left\{ v \in H^2(\Gamma) \mid (v, g_i)_{L^2(\Gamma)} = 0 \ \forall 1 \leq i \leq L \right\}.$$

The resulting minimisation problem, which we will discretise, is given as follows.

Problem 4.6.4. *Given $X \in \Gamma^N$ and $\delta, \rho > 0$ find $u_{\delta,\rho} \in H^2(\Gamma)$ minimising $\mathcal{E}_{\delta,\rho}(\cdot, X)$ over $H^2(\Gamma)$, where*

$$\mathcal{E}_{\delta,\rho}(u, X) := \frac{1}{2} a(u,u) + \frac{1}{2\delta} \sum_{i=1}^{N} (u(X_i) - \alpha_i)^2 + \frac{1}{2\rho} \sum_{i=1}^{L} (u, g_i)^2_{L^2(\Gamma)}.$$

Existence and uniqueness of a solution is a consequence of the Lax-Milgram theorem and by standard techniques for penalty methods one can show $\|u_{\delta,\rho} - u_\delta\|_{H^2(\Gamma)} \to 0$ as $\rho \to 0$, where u_δ is the solution to Problem 4.4.4. Here we will consider the case $\Gamma = T(1, \sqrt{2})$, a Clifford torus.

We discretise and solve the problem using the splitting $w = -\Delta_\Gamma u + u$. The resulting equations are as follows.

Problem 4.6.5. *Find $u_h, w_h \in \mathcal{S}_\langle$ such that for all $v_h \in \mathcal{S}_h$*

$$\left(t_h + \frac{1}{\delta}p_h + \frac{1}{\rho}k_h\right)(u_h, v_h) + (s_h + m_h)(w_h, v_h) = \frac{1}{\delta}\sum_{k=1}^{3} \alpha_k v_h^l(X_k),$$

$$(s_h + m_h)(u_h, v_h) - m_h(w_h, v_h) = 0.$$

Here m_h and s_h are the previously defined mass and stiffness operators respectively. The operator t_h is given by

$$\begin{aligned} t_h(u_h, v_h) = \int_{\Gamma_h} & \nabla_{\Gamma_h} u_h \cdot \left(\left[\frac{3}{2}H^2 - 2|\mathcal{H}|^2 - 2\right]\mathbb{1} - 2H\mathcal{H}\right)^{-l} \nabla_{\Gamma_h} v_h \\ & + u_h v_h \biggl(-\frac{3}{2}H^2|\mathcal{H}|^2 + 2(\nabla_\Gamma \nabla_\Gamma H) : \mathcal{H} + |\nabla_\Gamma H|^2 + 2HTr(\mathcal{H}^3) \\ & \qquad + \Delta_\Gamma |\mathcal{H}|^2 + |\mathcal{H}|^4 - 1\biggr)^{-l} \, do_h. \end{aligned}$$

This term in the equation results from discretising the remainder

$$t(u, v) = a(u, v) - \int_\Gamma (-\Delta_\Gamma u + u)(-\Delta_\Gamma v + v)\, do. \tag{4.39}$$

Note that the discretisation can only occur after integrating by parts to write $t(\cdot, \cdot)$ in an appropriate form. This calculation is performed in Lemma D.1.5. Now when we carry out the splitting $w = -\Delta_\Gamma u + u$ this expression becomes

$$a(u, v) = \int_\Gamma \nabla_\Gamma w \cdot \nabla_\Gamma v + wv\, do + t(u, v).$$

The operator p_h results from the penalty terms for the point constraints,

$$p_h(u_h, v_h) := \sum_{k=1}^{N} u_h^l(X_k) v_h^l(X_k).$$

The k_h term results from the penalty terms for the elements of $Ker(a)$,

$$k_h(u_h, v_h) := \sum_{k=1}^{L} \int_{\Gamma_h} u_h g_k^{-l} \, do_h \int_{\Gamma_h} v_h g_k^{-l} \, do_h.$$

The numerical analysis of this method will be the subject of the next chapter as it can be done in a more general setting which needs more notation than it is appropriate to introduce here. In this chapter we shall simply produce some illustrative examples.

Remark 4.6.1. *The point constraints problem may also be approached by adjusting the linear functionals $u \mapsto u(X_k)$ as was done for point forces in* (4.28)*. Similarly the point forces problem may be approached by a penalty method by penalising each of the integrals $(u, g_i)_{L^2(\Gamma)}$.*

4.6.7 Numerical results

We have chosen to study point constraints and point forces. Here we have studied the former on a sphere and the latter on a Clifford torus. This choice is arbitrary, the same methods can be applied to any combination of problem and surface.

Point forces on a sphere

As in the flat case (Chapter 2) we investigate the membrane mediated interactions between point forces. To do so we solve the discrete problem, Problem 4.6.1, with $R = 1$, $N = 2$, $X_1 = (0, 0, 1)$ and and $X_2 = (\sin(\theta), 0, \cos(\theta))$, varying $\theta \in [0, \pi]$. We take $\beta_1 = 5$ and consider each of the cases $\beta = \pm 5$. As in the flat case, we fix $\kappa = 1$ but use varying values for the surface tension σ to explore how the ratio κ/σ affects the interactions.

Figure 4.2a plots the energy of the discrete solution as a function of θ for point forces with the same sign, $\beta_1 = \beta_2 = 5$. At small separations we observe a similar attractive interaction as was observed in the flat case [31]. This agrees with the attractive interaction between filopodia discussed in biophysics literature [2, 44]. However there is a critical separation angle θ_c beyond which the interaction is repulsive. This repulsion at larger separations cannot be observed in the flat case as it occurs precisely when the membrane is no longer well approximated by a planar graph. The global minimum is at $\theta = 0$, corresponding to the two forces clustering to the same point as was observed in the flat case and proven by the general theory. There is also a local minimum at $\theta = \pi$, corresponding to the forces being located at opposite poles.

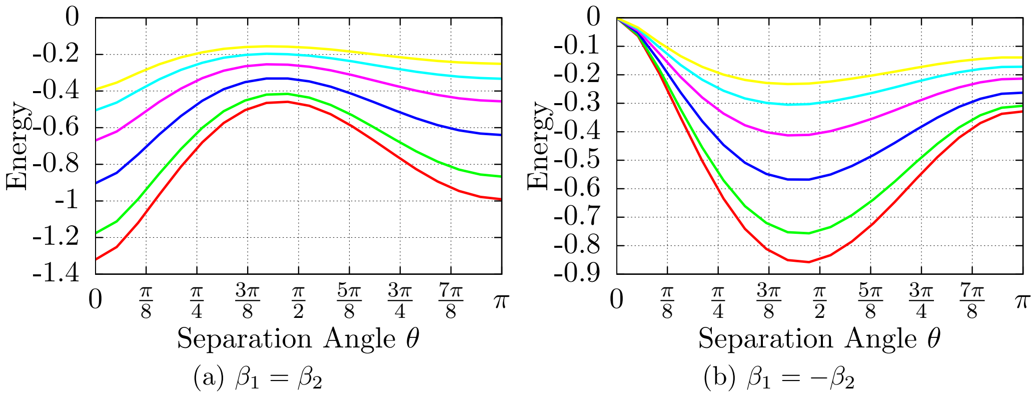


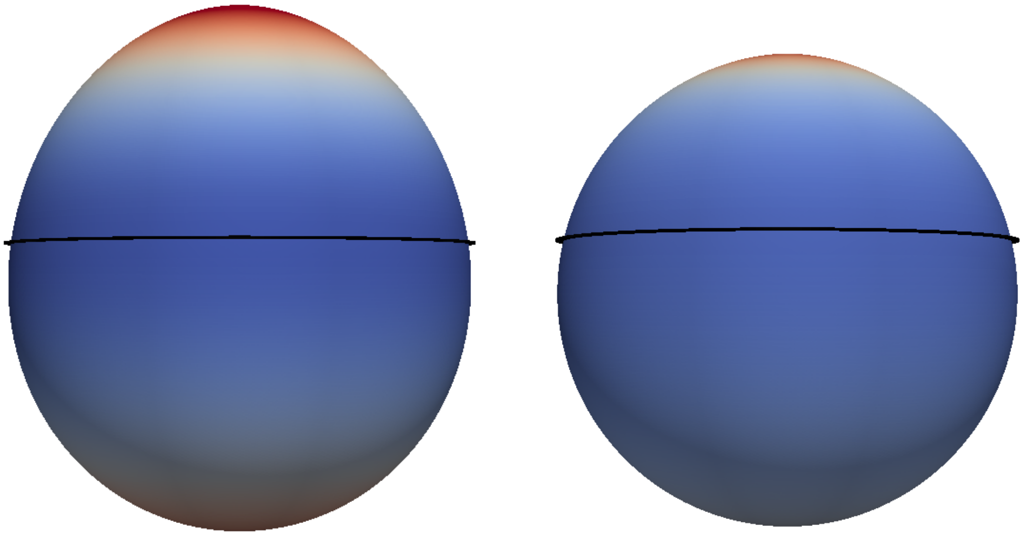
Figure 4.2: Energy plots for forces with identical and opposite orientations, varying σ from 0 to 25 (bottom to top).

Figure 4.2b plots the energy of the discrete solution as a function of θ for point forces with the opposite sign, $\beta_1 = -\beta_2 = 5$. At small separations we observe a similar repulsive interaction as was observed in the flat case. As for the previous example, the interaction changes at the critical angle θ_c, in this case becoming attractive. This leads to the global minimum occurring at $\theta = \theta_c$.

The existence of this critical angle and its dependence on σ can be seen by studying G_h, the solution for $N = 1$, $X_1 = (0, 0, 1)$ and $\beta = 1$. The θ-dependent part of the discrete energy for the two examples above may be written as

$$E_h(\theta) = -\beta_1 \beta_2 G_h(X_2(\theta)).$$

Thus when β_1 and β_2 have the same sign, the energy is least when $G_h > 0$ and when they have opposite sign the energy is least when $G_h < 0$. Moreover the critical angle θ_c is precisely the angle which minimises $G_h(X(\theta))$. Figure 4.3a plots G_h for $\sigma = 0$ and Figure 4.3b for $\sigma = 25$. The red regions are areas where G_h is positive and the blue where it is negative. The values are plotted onto a surface representative of the deformed surface G_h produces in each case. So that the deformations are visible, they have not been scaled by ε for these plots. Also overlayed on each figure is the line along which the minimum occurs, that is the line $\theta = \theta_c$. For $\sigma = 0$ we have $\theta_c \approx 83°$ and for $\sigma = 25$ we have $\theta_c \approx 77°$. One observes that as σ increases the effect of the force becomes more localised, shrinking the positive, red region and decreasing the value of θ_c.



(a) $\sigma = 0$ (b) $\sigma = 25$

Figure 4.3: Plot of G_h values on Γ_h for varying σ.

Point constraints for a Clifford torus

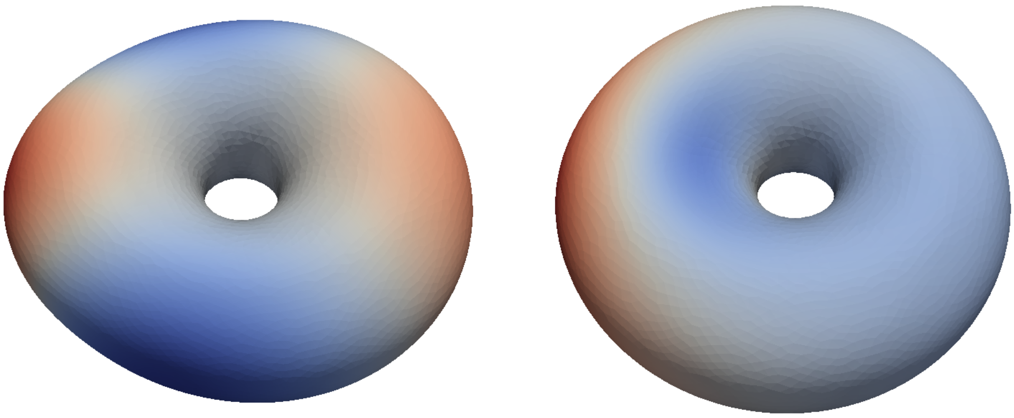
For the second algorithm we will simply provide some illustrative examples of numerical solutions. Figure 4.4a shows the deformed surface produced when minimising the linearised energy under the point constraints $u(X_k) = \alpha_i$ for $k = 1, 2, 3$ with

$$\begin{aligned} X_k &= ((\sqrt{2}+1)\cos((2+k)\pi/4), (\sqrt{2}+1)\sin((2+k)\pi/4), 0), \\ \alpha &= (-0.5, 1, -0.5). \end{aligned}$$

Figure 4.4b shows the deformed surface produced when minimising the linearised energy under the point constraints $u(X_k) = \alpha_i$ for $k = 1, 2, 3$ with

$$\begin{aligned} X_k &= (-(\sqrt{2}+\cos(2k\pi/3)), 0, \sin(2k\pi/3)), \\ \alpha &= (-0.5, -0.5, 1). \end{aligned}$$

In both cases there are deformations away from the point constraint locations. As for the point forces on a sphere, this will give rise to longer distance interactions that are not witnessed when the undeformed surface is planar. Note that the figures show the deformed surface Γ_ε, here we have chosen $\varepsilon = 0.2$. In reality ε is a much smaller parameter but using a relatively large value for ε in these plots means the deformations are visible.



(a) Constraints around outer circle (b) Constraints around inner cricle

Figure 4.4: Examples of deformed Clifford tori subject to point constraints.

Chapter 5

Second order splitting for a class of fourth order equations

5.1 Introduction

We will consider a coupled system of equations. This system is motivated by splitting methods in which we turn a single high order partial differential equation into a coupled system of lower order equations. For example consider the PDE

$$Au = f, \tag{5.1}$$

where A is a fourth order differential operator. Suppose we may write $A = B_1 \circ B_2 + C$, where B_1, B_2 and C are second order differential operators. By introducing a new variable, $w = B_2 u$, we may rewrite (5.1) as a coupled system of equations

$$\begin{aligned} Cu + B_1 w &= f, \\ B_2 u - w &= 0. \end{aligned} \tag{5.2}$$

The advantage of such a splitting method is that the resulting system of equations is second order, it can thus be solved numerically using simpler finite elements than are required to directly solve (5.1). To be an effective method however the system (5.2) must itself be well posed. This question is considered in [16], where sharp conditions are given detailing well posedness of the system. Amongst these conditions is a relationship between the norm of $B_1 - B_2$ and other properties of the operators (see [16, Section 3.1]). When designing a splitting method it can be difficult to ensure that this condition holds. To avoid this issue we will take $B_1 = B_2$, this case is studied in [47, 82]. These papers treat the case where C

induces a bilinear operator that is coercive or at least positive semi definite. We will not make this assumption here as it is not compatible with many of problems we wish to consider. To illustrate this point, consider the case

$$A = \Delta^2 u + \Delta u + u.$$

Such an A induces a coercive bilinear form on H^2 thus a problem of the form (5.1) is well posed. However to perform a splitting which satisfies the conditions in [47, 82] we require a B_1 which induces a bilinear form satisfying an inf sup condition, equivalently B_1 is invertible in an appropriate sense, and C which induces a positive semi-definite bilinear form. A reasonably general choice is $B_1 = -\Delta + \lambda$ for some $\lambda > 0$ but this produces

$$C = A - B_1 \circ B_1 = (1 + 2\lambda)\Delta + (1 - \lambda^2)$$

which isn't positive semi definite for any $\lambda > 0$. We will thus consider a situation where C does not induce a positive semi-definite bilinear form. Note that this work is not a direct generalisation of the results in [47, 82], whilst we consider a weaker condition on C this is accommodated by a stronger condition on the operator which acts on w in the second equation, chosen to be the negative identity map in (5.2).

5.2 Abstract splitting problem

We now introduce the coupled system on which the splitting method is based. Our abstract problem is formulated in a Banach space setting. We will first define the spaces and functionals used and the required assumptions.

Definition 5.2.1. *Let X, Y be reflexive Banach spaces and L be a Hilbert space with $Y \subset L$ continuously. Let $\{c,b,m\}$ be bilinear functionals such that*

$c : X \times X \to \mathbb{R}$, *bounded and bilinear,*

$b : X \times Y \to \mathbb{R}$, *bounded, bilinear and satisfies inf sup conditions,*

$m : L \times L \to \mathbb{R}$, *bounded, bilinear, symmetric and coercive.*

The inf sup conditions are that there exist $\beta, \gamma > 0$ such that

$$\beta \|\eta\|_X \leq \sup_{\xi \in Y} \frac{b(\eta, \xi)}{\|\xi\|_Y} \ \ \forall \eta \in X \quad \textit{and} \quad \gamma \|\xi\|_Y \leq \sup_{\eta \in X} \frac{b(\eta, \xi)}{\|\eta\|_X} \ \ \forall \xi \in Y. \tag{5.3}$$

We also assume the following relation between the bilinear forms, there exists $C > 0$

such that for all $(u, w) \in X \times Y$

$$b(u, \xi) = m(w, \xi) \; \forall \xi \in Y \implies C\|w\|_L^2 \leq c(u, u) + m(w, w). \tag{5.4}$$

Finally, let $f \in X^*$ *and* $g \in Y^*$*.*

Before formulating the full abstract problem we will return to the motivating example in (5.1) and (5.2), with $B_1 = B_2$, to justify the assumption (5.4). To formulate this problem in terms of Definition 5.2.1 we take $b, c : H^1(\Gamma) \times H^1(\Gamma) \to \mathbb{R}$ to be the weak forms of B_1 and C respectively. We then set $m : L^2(\Gamma) \times L^2(\Gamma) \to \mathbb{R}$ to be the standard L^2-inner product. We assume B_1 admits a $H^2(\Gamma)$ regularity property of the form

$$b(u, v) = m(w, v) \quad \forall v \in H^1(\Gamma) \implies u \in H^2(\Gamma) \text{ and } B_1 u = w.$$

This is a fairly standard property, for example it is satisfied by $B_1 = -\Delta_\Gamma + 1$. It then follows

$$m(w, w) + c(u, u) = m(B_1 u, B_1 u) + c(u, u) = a(u, u),$$

where $a : H^2(\Gamma) \times H^2(\Gamma) \to \mathbb{R}$ is the weak form of the fourth order operator A in (5.1). We assume a is coercive over $H^2(\Gamma)$, this is essentially assuming the underlying problem (5.1) is well posed. It follows

$$m(w, w) + c(u, u) \geq C_1 \|u\|_{H^2(\Gamma)} \geq C_2 \|w\|_{L^2(\Gamma)},$$

which is precisely the condition assumed in (5.4).

Using this general setting we formulate the coupled problem. Note that we allow a non-zero right hand side in each equation, this is a generalisation of the motivating problem (5.2).

Problem 5.2.1. *With the spaces and functionals in Definition 5.2.1, find* $(u, w) \in X \times Y$ *such that*

$$\begin{aligned} c(u, \eta) + b(\eta, w) &= \langle f, \eta \rangle \quad \forall \eta \in X, \\ b(u, \xi) - m(w, \xi) &= \langle g, \xi \rangle \quad \forall \xi \in Y. \end{aligned} \tag{5.5}$$

Before proving well posedness we will first give some context to this general problem within the existing literature. If we were to set $m = 0$ the resulting saddle point problem is well studied, see for example [32], and the assumptions we make on b and c are sufficient to show well posedness. The $m \neq 0$ case is examined in

[11, 16, 47]. There well posedness is shown under a different set of assumptions, only one of the inf sup conditions is required for b and m has a weaker coercivity assumption but c is assumed to be coercive. Note that these assumptions are weaker than the ones used in this work for b and m but stronger for c. Our assumptions are motivated by an application of this general theory to formulate a splitting method for the point forces and point constraints problems posed over a torus, see Problem 4.4.1 and Problem 4.4.4 in Chapter 4. The complexity of the fourth order operator we wish to split, which results from the second variation of the Willmore functional, makes it difficult to formulate the splitting problem in such a way that the existing theory can be applied. Such a formulation may be possible but it is our belief that the method presented here is more straightforward to apply to this and similar problems. Moreover the additional assumptions we make on b and m are quite natural for the applications we consider.

We now show the well posedness of this problem, the proof will make use of a generalised form of the Lax-Milgram theorem, the Banach-Nečas-Babuška Theorem [32, Section 2.1.3]. For completeness, the theorem is stated below.

Theorem 5.2.1 (Banach-Nečas-Babuška). *Let W be a Banach Space and let V be a reflexive Banach space. Let $A \in \mathcal{L}(W \times V; \mathbb{R})$ and $F \in V^*$. Then there exists a unique $u_F \in W$ such that*

$$A(u_F, v) = F(v) \;\; \forall v \in V$$

if and only if

$$\begin{aligned}
&\exists \alpha \geq 0 \;\; \forall w \in W, \quad \sup_{v \in V} \frac{A(w,v)}{\|v\|_V} \geq \alpha \|w\|_W, \\
&\forall v \in V, \quad (\forall w \in W, \; A(w,v) = 0) \implies v = 0.
\end{aligned}$$

Moreover the following a priori estimate holds

$$\forall F \in V^*, \quad \|u_F\|_W \leq \alpha^{-1} \|F\|_{V^*}.$$

For existence we will make the additional assumption that the spaces X and Y can be approximated by sequences of finite dimensional spaces. Moreover we assume that such approximating spaces are sufficiently rich to satisfy an appropriate inf sup inequality. This assumption allows us to use a Galerkin approach.

Definition 5.2.2. *We assume there exist sequences of finite dimensional approximating spaces $X_n \subset X$ and $Y_n \subset Y$. That is, for any $\eta \in X$ there exists a sequence*

$\eta_n \in X_n$ such that $\|\eta_n - \eta\|_X \to 0$, similarly for any $\xi \in Y$ there exists a sequence $\xi_n \in Y_n$ such that $\|\xi_n - \xi\|_Y \to 0$.

Moreover, we assume the discrete inf sup inequalities hold. That is there exist $\tilde{\beta}, \tilde{\gamma} > 0$, independent of n, such that

$$\tilde{\beta}\|\eta\|_X \leq \sup_{\xi \in Y_n} \frac{b(\eta,\xi)}{\|\xi\|_Y} \ \ \forall \eta \in X_n,$$
$$\tilde{\gamma}\|\xi\|_Y \leq \sup_{\eta \in X_n} \frac{b(\eta,\xi)}{\|\eta\|_X} \ \ \forall \xi \in Y_n.$$

Finally, assume there exists a map $I_n : Y \to Y_n$ for each n, such that

$$\begin{aligned} &b(\xi,\eta_n) = b(I_n\xi,\eta_n) \quad \forall(\xi,\eta_n) \in Y \times X_n,\\ &\sup_{\xi \in Y} \frac{\|\xi - I_n\xi\|_L}{\|\xi\|_Y} \to 0 \qquad \text{as } n \to \infty. \end{aligned} \tag{5.6}$$

Using these discrete inf sup inequalities and Theorem 5.2.1 we can construct a discrete inverse operator, this plays a key role in the proof of well posedness.

Lemma 5.2.1. *Under the assumptions of Definition 5.2.1 and Definition 5.2.2, there exists a linear map $G_n : Y^* \to X_n$ such that for each $\Theta \in Y^*$*

$$b(G_n\Theta, \xi_n) = \langle \Theta, \xi_n \rangle \ \ \forall \xi_n \in Y_n.$$

These maps satisfy the uniform bound

$$\|G_n\Theta\|_X \leq \tilde{\beta}^{-1}\|\Theta\|_{Y^*}.$$

Furthermore, there exists a map $G : Y^* \to X$ such that for each $\Theta \in Y^*$

$$b(G\Theta, \xi) = \langle \Theta, \xi \rangle \ \ \forall \xi \in Y.$$

This map satisfies the bound

$$\|G\Theta\|_{\mathcal{X}} \leq \beta^{-1}\|\Theta\|_{Y}.$$

Proof. To construct G_n, let $\Theta \in Y^*$, then $\Theta \in (Y_n, \|\cdot\|_Y)^*$. Then by Theorem 5.2.1, there exists a unique $G_n\Theta \in Y_n$ such that

$$b(G_n\Theta, \xi_n) = \langle \Theta, \xi_n \rangle \ \ \forall \xi_n \in Y_n.$$

The assumptions required to apply Theorem 5.2.1 are made in Definition 5.2.2.

That G_n is linear follows immediately from the construction. The two bounds are a consequence of the discrete inf sup inequalities in Definition 5.2.2. The map G is constructed similarly using the assumptions made in Definition 5.2.1. $\square$

We can now prove a discrete coercivity relation which is key in proving well posedness for Problem 5.2.1. This is a discrete analogue of (5.4).

Lemma 5.2.2. *Under the assumptions in Lemma 5.2.1, there exists $C, N > 0$ such that, for all $n \geq N$,*

$$C\|v_n\|_L^2 \leq c(G_n m(v_n, \cdot), G_n m(v_n, \cdot)) + m(v_n, v_n) \;\; \forall v_n \in Y_n. \tag{5.7}$$

Here $m(v_n, \cdot) \in Y^*$ denotes the map $y \mapsto m(v_n, y)$.

Proof. Let $v_n \in Y_n$, $m(v_n, \cdot) \in Y^*$ holds as Y is continuously embedded into L and observe

$$\|m(v_n, \cdot)\|_Y = \sup_{y \in Y} \frac{|m(v_n, y)|}{\|y\|_Y} \leq \frac{\|v_n\|_L \|y\|_L}{\|y\|_Y} \leq C\|v_n\|_L.$$

It follows, for any $\xi \in Y$,

$$\begin{aligned} b((G - G_n)m(v_n, \cdot), \xi) &= b((G - G_n)m(v_n, \cdot), \xi - I_n\xi), \\ &= b(Gm(v_n, \cdot), \xi - I_n\xi) \\ &= m(v_n, \xi - I_n\xi) \\ &\leq \|v_n\|_L \|\xi - I_n\xi\|_Y. \end{aligned}$$

Using the inf sup inequalities given in (5.3) we deduce

$$\|(G - G_n)m(v_n, \cdot)\|_X \leq C\|v_n\|_L \sup_{\xi \in Y} \frac{\|\xi - I_n\xi\|_L}{\|\xi\|_Y}.$$

For any $v_n \in Y_n$ we can thus bound the difference

$$|c(G_n m(v_n, \cdot), G_n m(v_n, \cdot)) - c(Gm(v_n, \cdot), Gm(v_n, \cdot))| \leq C\|v_n\|_L^2 \sup_{\xi \in Y} \frac{\|\xi - I_n\xi\|_L}{\|\xi\|_Y}.$$

Now, choosing n sufficiently large in the bound above, by (5.4) and (5.6) it follows for any $v_n \in Y_n$

$$C\|v_n\|_L^2 \leq c(G_n m(v_n, \cdot), G_n m(v_n, \cdot)) + m(v_n, v_n) + \frac{C}{2}\|v_n\|_L^2,$$

from which the result is immediate. $\square$

Theorem 5.2.2. *Suppose the assumptions of Definition 5.2.1 and Definition 5.2.2 hold, then there exists a unique solution to Problem 5.2.1. Moreover, there exists $C > 0$, independent of the data, such that*

$$\|u\|_X + \|w\|_Y \leq C(\|f\|_{X^*} + \|g\|_{Y^*}).$$

Proof. We begin with existence, using a Galerkin argument. Let $(u_n, w_n) \in X_n \times Y_n$ be the unique solution of

$$\begin{aligned} c(u_n, \eta_n) + b(\eta_n, w_n) &= \langle f, \eta_n \rangle \quad \forall \eta_n \in X_n, \\ b(u_n, \xi_n) - m(w_n, \xi_n) &= \langle g, \xi_n \rangle \quad \forall \xi_n \in Y_n. \end{aligned}$$

As the problem is linear and finite dimensional, existence and uniqueness of such a solution is equivalent to uniqueness for the homogeneous problem $f = g = 0$. In this case, testing the first equation with u_n, the second with w_n and subtracting we obtain

$$c(u_n, u_n) + m(w_n, w_n) = 0.$$

For sufficiently large n this implies $w_n = 0$ by (5.7), as $u_n = G_n m(w_n, \cdot)$ in the homogeneous case, thus $u_n = 0$ also, due to the linearity of G_n.

Now we return to the inhomogeneous case and produce a priori bounds on u_n, w_n. To create a pair of initial bounds we use the discrete inf sup inequalities with each of the finite dimensional equations. Firstly,

$$\tilde{\gamma}\|w_n\|_Y \leq \sup_{\eta_n \in X_n} \frac{b(\eta_n, w_n)}{\|\eta_n\|_X} \leq \|f\|_{X^*} + C\|u_n\|_X.$$

Similarly with the second equation,

$$\tilde{\beta}\|u_n\|_X \leq \sup_{\xi_n \in Y_n} \frac{b(u_n, \xi_n)}{\|\xi_n\|_Y} \leq \|g\|_{Y^*} + C\|w_n\|_L.$$

Combining these two inequalities produces

$$\|u_n\|_X + \|w_n\|_Y \leq C(\|f\|_{X^*} + \|g\|_{Y^*} + \|w_n\|_L). \tag{5.8}$$

To bound the $\|w_n\|_L$ term we use the same approach of subtracting the equations as used to show uniqueness. In the inhomogeneous case this produces

$$c(u_n, u_n) + m(w_n, w_n) = \langle f, u_n \rangle - \langle g, w_n \rangle.$$

Notice now $u_n = G_n m(w_n, \cdot) + G_n g$, thus

$$\begin{aligned} C\|w_n\|_L^2 &\leq c(u_n, u_n) + m(w_n, w_n) - c(u_n, G_n g) - c(G_n g, u_n) + c(G_n g, G_n g), \\ &\leq \|f\|_{X^*}\|u_n\|_X + \|g\|_{Y^*}\|w_n\|_Y + C(\|u_n\|_X + \|G_n g\|_X)\|G_n g\|_X. \end{aligned}$$

Recall, by Lemma 5.2.1,

$$\|G_n g\|_X \leq \tilde{\beta}^{-1}\|g\|_{Y^*}.$$

Combining these two inequalities with (5.8) produces

$$\|w_n\|_L^2 \leq C(\|f\|_{X^*} + \|g\|_{Y^*})(\|f\|_{X^*} + \|g\|_{Y^*} + \|w_n\|_L).$$

Hence by Young's inequality we deduce

$$\|w_n\|_L \leq C(\|f\|_{X^*} + \|g\|_{Y^*}),$$

then inserting this bound into (5.8) produces

$$\|u_n\|_X + \|w_n\|_Y \leq C(\|f\|_{X^*} + \|g\|_{Y^*}).$$

Thus u_n and w_n are bounded sequences in X and Y respectively, which are both reflexive Banach spaces, hence there exists a subsequence (which we continue to denote with a subscript n) such that

$$u_n \xrightharpoonup{X} u \quad \text{and} \quad w_n \xrightharpoonup{Y} w,$$

for some weak limits $u \in X$ and $w \in Y$. We will show that this weak limit is a solution to Problem 5.2.1. For any $\eta \in X$, there exists an approximating sequence $\eta_n \to \eta$ with each $\eta_n \in X_n$, it follows

$$c(u, \eta) + b(\eta, w) = \lim_{n\to\infty} c(u_n, \eta_n) + b(\eta_n, w_n) = \lim_{n\to\infty} \langle f, \eta_n \rangle = \langle f, \eta \rangle.$$

We treat the second equation similarly, for any $\xi \in Y$ we may find a sequence $\xi_n \to \xi$ with each $\xi_n \in Y_n$ and

$$b(u, \xi) - m(w, \xi) = \lim_{n\to\infty} b(u_n, \xi_n) - m(\xi_n, u_n) = \lim_{n\to\infty} \langle g, \xi_n \rangle = \langle g, \xi \rangle.$$

Thus (u, w) does indeed solve Problem 5.2.1. Moreover, as u, w are the weak limits of bounded sequences in reflexive Banach spaces their norms satisfy the same upper bound, that is

$$\|u\|_X + \|w\|_Y \leq C(\|f\|_{X^*} + \|g\|_{Y^*}).$$

We complete the proof by proving uniqueness, as the system is linear it is sufficient to consider the homogeneous case $f = g = 0$. In such a case $b(u, \xi) = m(w, \xi)\ \forall \xi \in Y$ and

$$c(u, u) + m(w, w) = 0.$$

Then by (5.4) we have $w = 0$ and hence $u = 0$. □

5.3 Applications to PDEs

5.3.1 Clifford torus problems

We now look to apply the above theory to produce a splitting method for a pair of fourth order problems, based around the second variation of the Willmore functional, posed on a Clifford torus $\Gamma = T(R, R\sqrt{2})$. The problems are derived and motivated in Chapter 4. Here we shall simply state them in terms of the abstract framework developed above.

Definition 5.3.1. *With respect to Definition 5.2.1, set the spaces to be $L = L^2(\Gamma)$, $X = W^{1,q}(\Gamma)$ and $Y = W^{1,p}(\Gamma)$, where $1 < p' < p < 2 < q < q' < \infty$ such that $1/p + 1/q = 1$ and $1/p' + 1/q' = 1$. Let $\delta, \rho > 0$ be sufficiently small. We set the bilinear functionals to be as follows,*

$$\begin{aligned}
r_1(u, v) :=& \frac{1}{\rho} \sum_{k=1}^{K} \int_\Gamma u g_k \, do \int_\Gamma v g_k \, do + \chi_{con} \frac{1}{\delta} \sum_{k=1}^{N} u(X_k) v(X_k), \\
r_2(u, v) :=& \int_\Gamma \nabla_\Gamma u \cdot \left(\left[\frac{3}{2} H^2 - 2|\mathcal{H}|^2 - 2 \right] \mathbb{1} - 2H\mathcal{H} \right) \nabla_\Gamma v \\
&+ uv \left(-\frac{3}{2} H^2 |\mathcal{H}|^2 + 2(\nabla_\Gamma \nabla_\Gamma H) : \mathcal{H} + |\nabla_\Gamma H|^2 + 2HTr(\mathcal{H}^3) + \Delta_\Gamma |\mathcal{H}|^2 + |\mathcal{H}|^4 - 1 \right) do, \\
c(u, v) :=& r_1(u, v) + r_2(u, v), \\
b(u, v) :=& \int_\Gamma \nabla_\Gamma u \cdot \nabla_\Gamma v + uv \, do, \\
m(v, w) :=& \int_\Gamma vw \, do.
\end{aligned}$$

Here $\chi_{con} = 0$ or 1 for the point forces or point constraints problem respectively. The functions g_k are smooth and form a basis for the kernel of the second variation of the Willmore functional. Their specific form is given in Chapter 4 but is not *required here. Finally set $g = 0$ and f such that*

$$\langle f, v\rangle = \sum_{k=1}^{N} \beta_k v(X_k) \quad \text{or} \quad \langle f, v\rangle = \frac{1}{\delta}\sum_{k=1}^{N} \alpha_k v(X_k),$$

for the point forces or point constraints problem respectively.

Observe that the bilinear form $r_2(\cdot,\cdot)$ is precisely the remainder term $t(\cdot,\cdot)$ defined in (4.39). We will now check that all of the assumptions required in Definition 5.2.1 hold for the choices made above in Definition 5.3.1. Most of these are straightforward however the inf sup conditions require the following proposition.

Proposition 5.3.1. *Suppose $1 < p \leq 2 \leq q < \infty$ are chosen such that $1/p + 1/q = 1$. Let $\lambda > 0$, $X = W^{1,q}(\Gamma)$, $Y = W^{1,p}(\Gamma)$ and $b : X \times Y \to \mathbb{R}$ be given by*

$$b(u, v) := \int_\Gamma \nabla_\Gamma u \cdot \nabla_\Gamma v + \lambda uv \, do.$$

There exist $\beta, \gamma > 0$ such that

$$\beta \|\eta\|_X \leq \sup_{\xi \in Y} \frac{b(\eta,\xi)}{\|\xi\|_Y} \ \ \forall \eta \in X \quad \text{and} \quad \gamma\|\xi\|_Y \leq \sup_{\eta\in X}\frac{b(\eta,\xi)}{\|\eta\|_X} \ \ \forall \xi \in Y.$$

Proof. Consider the map $A : W^{1,p}(\Gamma) \to W^{1,q}(\Gamma)^*$ given, for each $u \in W^{1,p}(\Gamma)$ by

$$A(u)[v] := b(v, u).$$

Evidently A is well-defined and linear, by Hölder's inequality it is also continuous. We will now show that it is an isomorphism, beginning with showing that A is surjective. Consider the inverse Laplacian type map $T : L^2(\Gamma) \to H^2(\Gamma)$, defined by $Tf \in H^2(\Gamma)$ is the unique solution to

$$b(Tf, v) = \int_\Gamma fv \quad \forall v \in H^1(\Gamma).$$

That T is well defined, continuous and a bijection follows by elliptic regularity. It is immediate that $T^{-1} = -\Delta_\Gamma + \lambda Id$. Now suppose $F \in W^{1,q}(\Gamma)^*$ and set $g := T^*(F) \in L^2(\Omega)$, this is well defined as $H^2(\Gamma)^* \subset W^{1,q}(\Gamma)^*$. For any $\varphi \in C_0^\infty(\Gamma)$ and first order derivative $\underline{D}_\alpha$ it holds

$$\begin{aligned}
&\int_\Gamma g\underline{D}_\alpha \varphi = \int_\Gamma g\underline{D}_\alpha T^{-1}T\varphi, \\
&= \int_\Gamma g\left(T^{-1}\underline{D}_\alpha T\varphi + \nu_\alpha(2\mathcal{H} : \nabla_\Gamma\nabla_\Gamma T\varphi + \nabla_\Gamma H \cdot \nabla_\Gamma T\varphi) + \left[(2\mathcal{H}^2 - H\mathcal{H})\nabla_\Gamma T\varphi\right]_\alpha\right).
\end{aligned}$$

The second line is due to a commutation relation for $\underline{D}_\alpha$ and Δ_Γ which follows from [27, Lemma 2.6]. It then follows

$$\begin{aligned}&\int_\Gamma -g\underline{D}_\alpha\varphi + H\nu_\alpha gT\varphi\\ &= \langle F, T\left(H\nu_\alpha T\varphi - \nu_\alpha(2\mathcal{H} : \nabla_\Gamma\nabla_\Gamma T\varphi + \nabla_\Gamma H\cdot\nabla_\Gamma T\varphi) - \left[(2\mathcal{H}^2 - H\mathcal{H})\nabla_\Gamma T\varphi\right]_\alpha\right)\rangle\\ &\quad - \langle F, \underline{D}_\alpha T\varphi\rangle.\end{aligned}$$

Notice $T \in \mathcal{L}(L^q(\Gamma), W^{2,q}(\Gamma))$, $\underline{D}_\alpha \in \mathcal{L}(W^{2,q}(\Gamma), W^{1,q}(\Gamma))$ and thus thus we may extend the map $\varphi \mapsto -\langle F, \underline{D}_\alpha T\varphi\rangle$ to $L^q(\Gamma)$ and that extension lies in $L^q(\Gamma)^*$. The second term may be treated in a similar manner. It follows there exists $g_\alpha \in L^p(\Gamma)$ such that

$$\int_\Gamma -g\underline{D}_\alpha\varphi + H\nu_\alpha gT\varphi = \int_\Gamma g_\alpha\varphi \quad \forall\varphi \in C_0^\infty(\Gamma).$$

Hence $g \in W^{1,p}(\Gamma)$. Now, for the constructed $g \in W^{1,p}(\Gamma)$ it holds, for any $v \in H^2(\Gamma)$,

$$\int_\Omega g(-\Delta v + \lambda v) = \int_\Omega T^*FT^{-1}v = \langle F, v\rangle.$$

Integrating the left hand side by parts and using density the above equation implies, for any $v \in W^{1,q}(\Gamma)$,

$$A(g)[v] = \int_\Omega \nabla_\Gamma g\cdot\nabla_\Gamma v + \lambda gv = \langle F, v\rangle.$$

Hence $A(g) = F$ and thus A is surjective. To show A is injective, suppose $A(u) = 0$, then in particular,

$$0 = A(u)[Tu] = \int_\Gamma u^2 \implies u = 0.$$

Thus A is a bijection and by the bounded inverse theorem A^{-1} is also bounded, it follows

$$\|\eta\|_X \le \|A^{-1}\|\|A\eta\|_{Y^*} \quad \forall\eta \in X.$$

Hence we obtain

$$\|A^{-1}\|^{-1}\|\eta\|_X \le \sup_{\xi\in Y}\frac{b(\eta,\xi)}{\|\xi\|_Y}.$$

Additionally, $(A^*)^{-1} = (A^{-1})^*$ is bounded, thus similarly

$$\|(A^*)^{-1}\|^{-1}\|\xi\|_Y \le \sup_{\eta\in X}\frac{A^*(\xi)[\eta]}{\|\eta\|_X}.$$

Finally notice $A^*(\xi)[\eta] = A(\eta)[\xi] = b(\eta,\xi)$, completing the second inf sup inequality.

$\square$

Now we check the remaining assumptions required.

Lemma 5.3.1. *The assumptions made in Definition 5.2.1 hold for the choices made for the spaces and functionals in Definition 5.3.1.*

Proof. The space $L^2(\Gamma)$ is a Hilbert Space and $W^{1,r}(\Gamma)$ is a reflexive Banach space for any $1 < r < \infty$. The embeddings $W^{1,p}(\Gamma) \subset W^{1,p'}(\Gamma) \subset L^2(\Gamma)$ and $W^{1,q'}(\Gamma) \subset W^{1,q}(\Gamma)$ are continuous by the Sobolev embedding theorem.

Having proven the inf sup inequalities in Proposition 5.3.1, the remaining conditions on c, r, b and m are straightforward. To obtain the coercivity relation (5.4), in this case

$$b(u,\xi) = m(w,\xi)\ \forall \xi \in Y \implies u \in H^2(\Gamma) \text{ and } w = -\Delta_\Gamma u + u.$$

It follows, using the fact that $r_2 = t$, defined in (4.39),

$$c(u,u) + m(w,w) = \int_\Gamma (\Delta_\Gamma u)^2 + 2|\nabla_\Gamma u|^2 + u^2 + c(u,u) \geq C\|u\|_{2,2}^2 \geq C\|w\|_{0,2}^2.$$

The H^2 coercivity result used here holds for sufficiently small δ, ρ and is proven in Chapter 4.

Finally, the choices for f and g lie in the required dual spaces. For f this follows from the continuous embedding $W^{1,q}(\Gamma) \subset C^0(\Gamma)$. $\square$

We now introduce the lifted discrete spaces, they will satisfy the assumptions required in Definition 5.2.2 for this application. We will use standard the lift operator as constructed in [27, Section 4.1]. The lifted discrete spaces satisfy the conditions in Definition 5.2.2 when we set $X_n = Y_n = \mathcal{S}_h^l$ and $h = 1/n$. For the approximation and uniform convergence conditions (5.6) we will make use of the Ritz projection which is defined in the lemma below.

Lemma 5.3.2. *Suppose $\lambda > 0$, let $1 < r < \infty$ and $b : W^{1,r}(\Gamma) \times W^{1,s}(\Gamma) \to \mathbb{R}$ given by*

$$b(u,v) := \int_\Gamma \nabla_\Gamma u \cdot \nabla_\Gamma v + \lambda uv \, do,$$

where $1 < s < \infty$ is chosen such that $1/r + 1/s = 1$. For each $h > 0$, there exists a bounded linear map $\Pi_h : W^{1,r}(\Gamma) \to (\mathcal{S}_h^l, \|\|_{1,r})$ given by

$$b(\Pi_h \psi, v_h^l) = b(\psi, v_h^l) \quad \forall v_h \in \mathcal{S}_h.$$

There exists $C(r) > 0$, independent of h, such that

$$\|\Pi_h \psi\|_{1,r} \leq C(r)\|\psi\|_{1,r} \quad \forall \psi \in W^{1,r}(\Gamma).$$

Finally, it holds

$$\sup_{\psi \in W^{1,r}(\Gamma)} \frac{\|\psi - \Pi_h \psi\|_{0,2}}{\|\psi\|_{1,r}} \to 0 \text{ as } h \to 0.$$

Proof. One can see the Ritz projection, Π_h is well defined as this is equivalent to the invertibility of $S + \lambda M$, where S, M are the usual mass and stiffness matrices for lifted finite elements. Linearity is then immediate from the definition. To begin the proof of continuity we first consider $2 \leq r < \infty$. We also consider the similar projection $\mathcal{P}_h : W^{1,r}(\Gamma) \to \mathcal{S}_h^l$ such that

$$\int_{\Gamma_h} \nabla_{\Gamma_h} \mathcal{P}_h^{-l} \psi \cdot \nabla_{\Gamma_h} v_h + \lambda \mathcal{P}_h^{-l} \psi v_h \, do_h = b(\psi, v_h^l) \quad \forall v_h \in \mathcal{S}_h.$$

Using [50, Theorem 3.1, Lemma 3.8], for any $2 \leq r < \infty$ there exists $C(r) > 0$, independent of h, such that

$$\|\mathcal{P}_h \psi\|_{1,r} \leq C(r)\|\psi\|_{1,r} \quad \forall \psi \in W^{1,r}(\Gamma).$$

This is proven for $r = 2$ and $r = \infty$ in [50], the above result then follows by interpolating between the two spaces. By density $\mathcal{P}_h$ may be extended to $\psi \in W^{1,r}(\Gamma)$ for $1 < r < 2$. Furthermore for any $v \in W^{1,s}(\Gamma)$,

$$b(\mathcal{P}_h \psi, v) = b_h(\mathcal{P}_h^{-l} \psi, \mathcal{P}_h^{-l} v) = b(\psi, \mathcal{P}_h v) \leq C(s)\|\psi\|_{1,r}\|v\|_{1,s}.$$

Hence by Proposition 5.3.1 we may extend continuity for $\mathcal{P}_h$ to $1 < r < 2$,

$$\|\mathcal{P}_h \psi\|_{1,r} \leq C(t)\|\psi\|_{1,r} \quad \forall \psi \in W^{1,r}(\Gamma).$$

Also observe, arguing as in [50, Lemma 3.7], for any $1 < r < \infty$ it holds

$$b(\psi - \mathcal{P}_h \psi, v_h^l) \leq C\|\psi\|_{1,r}\|v_h^l\|_{1,s} \quad \forall (\psi, v_h) \in W^{1,r}(\Gamma) \times \mathcal{S}_h.$$

We may now prove a bound on the difference between the two projections. For any $v \in W^{1,s}(\Gamma)$ it holds

$$\begin{aligned} b(\Pi_h \psi - \mathcal{P}_h \psi, v) &= b(\Pi_h \psi - \mathcal{P}_h \psi, v - \mathcal{P}_h v) + b(\psi - \mathcal{P}_h \psi, \mathcal{P}_h v) \\ &\leq Ch^2(\|\Pi_h \psi - \mathcal{P}_h \psi\|_{1,r} + \|\psi\|_{1,r})\|v\|_{1,s}. \end{aligned}$$

Hence, using the inf sup inequalities proven in Proposition 5.3.1,

$$\|\Pi_h\psi - \mathcal{P}_h\psi\|_{1,r} \leq Ch^2\|\psi\|_{1,r}.$$

Thus it follows

$$\|\Pi_h\psi\|_{1,r} \leq \|\Pi_h\psi - \mathcal{P}_h\psi\|_{1,r} + \|\mathcal{P}_h\psi\|_{1,r} \leq C\|\psi\|_{1,r}.$$

For the final condition we will use the following interpolation estimate, for $2 \leq r < \infty$,

$$\inf_{v_h \in V_h} \|\psi - v_h\|_{1,r} \leq Ch^{2/r}\|\psi\|_{2,2} \quad \forall \psi \in H^2(\Gamma). \tag{5.9}$$

This result follows from [15, Theorem 3.1.6]. The calculation is as follows, denoting the interpolation operator by I_h and Sobolev norms over triangular elements $K \subset \mathcal{T}_h$ by $\|\cdot\|_{k,p,K}$. Firstly we decompose the surface Γ into curved triangles and move onto the discrete surface Γ_h using [27, Lemma 4.2].

$$\begin{aligned}
\|\psi - I_h\psi\|_{1,r} &= \left(\sum_{K\in\mathcal{T}_h} \|\psi - I_K\psi\|^r_{1,r,K}\right)^{1/r} \\
&\leq C\left(\sum_{K\in\mathcal{T}_h} |K|^{1-r/2}h^r\|\psi\|^r_{2,2,K}\right)^{1/r}
\end{aligned}$$

As $Ch^2 \leq |K|$ it follows $|K|^{1-r/2} \leq Ch^{2-r}$ and hence

$$\begin{aligned}
\|\psi - I_h\psi\|_{1,r} &\leq Ch^{2/r}\left(\sum_{K\in\mathcal{T}_h} \|\psi\|^r_{2,2,K}\right)^{1/r} \\
&\leq Ch^{2/r}\left(\sum_{K\in\mathcal{T}_h} \|\psi\|^2_{2,2,K}\right)^{1/2} \\
&\leq Ch^{2/r}\|\psi\|_{2,2}.
\end{aligned}$$

The penultimate line is due to the embedding of $\ell^r \subset \ell^2$ for $r \geq 2$ and the final line by moving back to the surface Γ, again using [27, Lemma 4.2]. We have thus shown (5.9).

Now, for any $\psi \in W^{1,r}(\Gamma)$, suppose $\varphi \in H^2(\Gamma)$ such that

$$b(\varphi, v) = \int_\Gamma (\psi - \Pi_h\psi) v \, do \quad \forall v \in H^1(\Gamma).$$

It follows

$$\|\psi - \Pi_h\psi\|_{0,2}^2 = b(\varphi, \psi - \Pi_h\psi) = b(\varphi - v_h^l, \psi - \Pi_h\psi),$$

where $v_h \in \mathcal{S}_h$ is arbitrary, hence for $2 \le r < \infty$,

$$\|\psi - \Pi_h\psi\|_{0,2}^2 \le Ch^{2/s}\|\varphi\|_{2,2}\|\psi\|_{1,r} \le Ch^{2/s}\|\psi - \Pi_h\psi\|_{0,2}\|\psi\|_{1,r}.$$

Similarly, for $1 < r < 2$,

$$\|\psi - \Pi_h\psi\|_{0,2}^2 \le \inf_{v_h \in \mathcal{S}_h} \|\varphi - v_h^l\|_{1,2}\|\psi\|_{1,2} \le Ch\|\psi - \Pi_h\psi\|_{0,2}\|\psi\|_{1,r}. \tag{5.10}$$

Hence, for any $1 < r < \infty$,

$$\sup_{\psi \in W^{1,r}(\Gamma)} \frac{\|\psi - \Pi_h\psi\|_{0,2}}{\|\psi\|_{1,r}} \to 0 \text{ as } h \to 0.$$

□

To prove the discrete inf sup conditions we require Fortin's criterion. We use the following form of the criterion, which follows from [32, Lemma 4.19].

Lemma 5.3.3. *Suppose V and W are Banach spaces and $\tilde{b} \in \mathcal{L}(V \times W; \mathbb{R})$ such that there exists $\beta > 0$ such that*

$$\beta \le \inf_{\xi \in W \setminus \{0\}} \sup_{\eta \in V \setminus \{0\}} \frac{\tilde{b}(\eta, \xi)}{\|\eta\|_V \|\xi\|_W}.$$

Let $V_h \subset V$ and $W_h \subset W$ with W_h reflexive. If there exists $\delta > 0$ such that, for all $\eta \in V$, there exists $\Pi_h(\eta) \in V_h$ such that

$$\forall \xi_h \in W_h, \quad \tilde{b}(\eta, \xi_h) = \tilde{b}(\Pi_h(\eta), \xi_h) \text{ and } \|\Pi_h(\eta)\|_V \le \delta \|\eta\|_V,$$

then

$$\frac{\beta}{\delta} \le \inf_{\xi_h \in W_h \setminus \{0\}} \sup_{\eta_h \in V_h \setminus \{0\}} \frac{\tilde{b}(\eta_h, \xi_h)}{\|\eta_h\|_V \|\xi_h\|_W}.$$

We can now prove the discrete inf sup conditions for $b(\cdot, \cdot)$.

Lemma 5.3.4. *Under the assumptions of Lemma 5.3.2, there exist $\tilde{\beta}, \tilde{\gamma} > 0$, independent of h, such that*

$$\tilde{\beta}\|\eta_h^l\|_{1,r} \leq \sup_{\xi_h \in \mathcal{S}_h} \frac{b(\eta_h^l, \xi_h^l)}{\|\xi_h^l\|_{1,s}} \;\; \forall \eta_h \in \mathcal{S}_h \quad \textit{and} \quad \tilde{\gamma}\|\xi_h^l\|_{1,s} \leq \sup_{\eta_h \in \mathcal{S}_h} \frac{b(\eta_h^l, \xi_h^l)}{\|\eta_h^l\|_{1,r}} \;\; \forall \xi_h \in \mathcal{S}_h.$$

Proof. We apply Fortin's Criterion (Lemma 5.3.3). Setting $V = W^{1,r}(\Gamma)$, $W = W^{1,s}(\Gamma)$, $V_h = W_h = \mathcal{S}_h$ and using the Ritz projection Π_h constructed above in Lemma 5.3.2 proves the first inf sup inequality. Similarly, setting $W = W^{1,r}(\Gamma)$ and $V = W^{1,s}(\Gamma)$ proves the reversed inf sup inequality. □

The splitting method is thus well posed, this follows by applying the abstract theory.

Corollary 5.3.1. *There exists a unique solution to Problem 5.2.1 with the spaces and functionals as chosen in Definition 5.3.1. Moreover we have the additional regularity $u \in W^{3,p}(\Gamma)$ for all $1 < p < 2$ and the regularity estimate*

$$\|u\|_{3,p} \leq C(p)\|w\|_{1,p}.$$

Proof. We have proven that the assumptions made in Definition 5.2.1 and Definition 5.2.2 hold in this case, thus we may apply Theorem 5.2.2 to show well posedness. The regularity result follows by elliptic regularity, applied to the second equation of the system. □

5.3.2 General fourth order problem

In the section we apply the abstract theory to splitting a fairly general fourth order surface PDE. That is we consider solving a problem of the form

$$\Delta_\Gamma^2 u - \nabla_\Gamma \cdot (\mathcal{B}\nabla_\Gamma u) + H\mathcal{B}\nabla_\Gamma u \cdot \nu + \mathcal{C}u = \mathcal{F},$$

posed over $\Gamma \subset \mathbb{R}^3$, a compact 2-dimensional smooth hypersurface. This PDE results from minimising the functional

$$\int_\Gamma (\Delta_\Gamma u)^2 + |\mathcal{B}\nabla_\Gamma u|^2 + \mathcal{C}u^2 \, do$$

over $H^2(\Gamma)$. If Γ is a planar domain, so $H = 0$, the resulting PDE is a generic fourth order problem once we fix some appropriate boundary conditions, for example $u = \Delta u = 0$ on $\partial\Omega$. We will make assumptions on $\mathcal{B}$ and $\mathcal{C}$ to ensure that the equation is well posed. This is done in the following weak formulation of the problem.

Problem 5.3.1. *Find $u \in H^2(\Gamma)$ such that*

$$\int_\Gamma \Delta_\Gamma u \Delta_\Gamma v + \mathcal{B}\nabla_\Gamma u \cdot \nabla_\Gamma v + \mathcal{C}uv \, do = \int_\Gamma \mathcal{F}v \, do \;\; \forall v \in H^2(\Gamma).$$

Where $\mathcal{C}(x) \in \mathbb{R}$ for all $x \in \Gamma$ and there exist $\mathcal{C}_m, \mathcal{C}_M > 0$ such that

$$\mathcal{C}_m < \mathcal{C}(x) < \mathcal{C}_M \;\; \forall x \in \Gamma.$$

We also assume that $\mathcal{B}(x) \in \mathbb{R}^{3\times 3}$ is symmetric for each $x \in \Gamma$ and there exists $\lambda_M > 0$ such that

$$\|\mathcal{B}(x)\| \leq \lambda_M \; \forall x \in \Gamma.$$

Further assume there exists $\Lambda > 0$ such that

$$\frac{\Lambda\lambda_M}{2} < \mathcal{C}_m \quad \text{and} \quad \frac{\lambda_M}{2\Lambda} < 1.$$

Finally we suppose $\mathcal{F} \in L^2(\Gamma)$.

The assumptions we make on $\mathcal{B}$ and $\mathcal{C}$ ensure that the bilinear functional is coercive and hence the problem is well posed by the Lax-Milgram theorem. Here we have chosen an L^2 right hand side, one could make a more general choice however we restrict to L^2 here as we will later show that in this case the numerical method attains the optimal order of convergence. We will now formulate an appropriate splitting method whose solution coincides with that of the fourth order problem.

Definition 5.3.2. *With respect to Definition 5.2.1, set $L = L^2(\Gamma)$, $X = Y = H^1(\Gamma)$. Set the bilinear functionals*

$$\begin{aligned}
c(u,v) &:= \int_\Gamma (\mathcal{B} - 2\mathbb{1})\nabla_\Gamma u \cdot \nabla_\Gamma v + (\mathcal{C} - 1)\, uv \, do, \\
b(u,v) &:= \int_\Gamma \nabla_\Gamma u \cdot \nabla_\Gamma v + uv \, do, \\
m(u,v) &:= \int_\Gamma uv \, do.
\end{aligned}$$

Finally, take the data to be

$$f := m(\mathcal{F}, \cdot) \qquad \text{and} \qquad g := m(\mathcal{G}, \cdot),$$

with $\mathcal{F}, \mathcal{G} \in L^2(\Gamma)$.

We can now use the abstract theory to show well posedness for this problem.

Proposition 5.3.2. *There exists a unique solution to Problem 5.2.1 with the spaces and functionals as chosen in Definition 5.3.2. Moreover we have the regularity result* $u, w \in H^2(\Gamma)$ *with the estimate*

$$\|u\|_{H^2(\Gamma)} + \|w\|_{H^2(\Gamma)} \leq C \left(\|\mathcal{F}\|_{L^2(\Gamma)} + \|\mathcal{G}\|_{L^2(\Gamma)} \right).$$

Furthermore, when $\mathcal{G} = 0$ *the solution* u *coincides with the solution of Problem 5.3.1.*

Proof. For the well posedness we apply Theorem 5.2.2. The assumptions required in Definition 5.2.1 are straightforward to check, firstly the inf sup conditions conditions are established in Proposition 5.3.4. For the coercivity relation (5.4) notice that

$$b(u, \xi) = m(w, \xi) \ \forall \xi \in Y \implies u \in H^2(\Gamma) \text{ and } w = -\Delta_\Gamma u + u,$$

hence we deduce

$$c(u, u) + m(w, w) = \int_\Gamma (\Delta_\Gamma u)^2 + \mathcal{B} \nabla_\Gamma u \cdot \nabla_\Gamma u + \mathcal{C} u^2 \, do \geq C\|u\|_{2,2} \geq C\|w\|_{0,2}.$$

For the assumptions made in Definition 5.2.2, we take the lifted discrete spaces described in the previous section and the required discrete inf sup inequalities again follow by Proposition 5.3.4. Finally, (5.6) holds by the same argument as used in the previous example using the Ritz projection in Lemma 5.3.2.

We thus have well posedness by Theorem 5.2.2. The regularity estimate follows by applying elliptic regularity to each of the equations of the system. Finally, when $\mathcal{G} = 0$, by elliptic regularity we have $w = -\Delta_\Gamma u + u$. It follows, for any $v \in H^2(\Gamma)$,

$$\int_\Gamma \mathcal{F} v \, do = (c + r)(u, v) + b(w, v) = \int_\Gamma \Delta_\Gamma u \Delta_\Gamma v + \mathcal{B} \nabla_\Gamma u \cdot \nabla_\Gamma v + \mathcal{C} uv \, do.$$

□

5.4 Abstract finite element method

In this section we lay out an abstract finite element method to approximate the solution of Problem 5.2.1. In our applications we wish to use a non-conforming finite element method as we will approximate problems based on a surface Γ via problems based on a discrete surface Γ_h. We will first introduce the abstract version of such a finite element method.

Definition 5.4.1. *In the setting of Definition 5.2.1, suppose, for $h > 0$, X_h, Y_h are finite dimensional normed vector spaces and there exist lift operators*

$$l_h^X : X_h \to X \quad \text{and} \quad l_h^Y : Y_h \to M,$$

which are linear and injective, such that $X_h^l := l_h^X(X_h)$ and $Y_h^l := l_h^Y(Y_h)$ satisfy Definition 5.2.2. For $\eta_h \in X_h$ let $\eta_h^l := l_h^X(\eta_h) \in X_h^l$, similarly for $\xi_h \in Y_h$ let $\xi_h^l := l_h^M(\xi_h) \in Y_h^l$.

Let c_h, b_h, m_h denote bilinear functionals such that

$$\begin{aligned}
&c_h : X_h \times X_h \to \mathbb{R}, \text{ bilinear},\\
&b_h : X_h \times Y_h \to \mathbb{R}, \text{ bilinear},\\
&m_h : Y_h \times Y_h \to \mathbb{R}, \text{ bilinear and symmetric}.
\end{aligned}$$

We will assume the following approximation properties, there exists $C, k > 0$ such that

$$\begin{aligned}
|c(\eta_h^l, \psi_h^l) - c_h(\eta_h, \psi_h)| &\leq Ch^k \|\eta_h^l\|_X \|\psi_h^l\|_X \quad \forall (\eta_h, \xi_h) \in X_h \times X_h,\\
|b(\eta_h^l, \xi_h^l) - b_h(\eta_h, \xi_h)| &\leq Ch^k \|\eta_h^l\|_X \|\xi_h^l\|_Y \quad \forall (\eta_h, \xi_h) \in X_h \times Y_h,\\
|m(\eta_h^l, \xi_h^l) - m_h(\eta_h, \xi_h)| &\leq Ch^k \|\eta_h^l\|_L \|\xi_h^l\|_L \quad \forall (\eta_h, \xi_h) \in Y_h \times Y_h.
\end{aligned}$$

Finally, let $f_h \in X_h^*$ and $g_h \in Y_h^*$, the dual spaces of X_h and Y_h respectively, be such that

$$\begin{aligned}
|\langle f, \eta_h^l \rangle - \langle f_h, \eta_h \rangle| &\leq Ch^k \|f\|_{X^*} \|\eta_h^l\|_X \quad \forall \eta_h \in X_h,\\
|\langle g, \xi_h^l \rangle - \langle g_h, \xi_h \rangle| &\leq Ch^k \|g\|_{Y^*} \|\xi_h^l\|_Y \quad \forall \xi_h \in Y_h.
\end{aligned}$$

The finite element approximation can now be formulated.

Problem 5.4.1. *Under the assumptions of Definition 5.4.1, find $(u_h, w_h) \in X_h \times Y_h$ solving the discretised problem*

$$\begin{aligned}
c_h(u_h, \eta_h) + b_h(\eta_h, w_h) &= \langle f_h, \eta_h \rangle \quad \forall \eta_h \in X_h,\\
b_h(u_h, \xi_h) - m_h(w_h, \xi_h) &= \langle g_h, \xi_h \rangle \quad \forall \xi_h \in Y_h.
\end{aligned}$$

We now prove well posedness for the finite element method, Problem 5.4.1, and produce a priori bounds for the solution.

Theorem 5.4.1. *For sufficiently small h, there exists a unique solution to Problem*

5.4.1. Moreover, there exists a constant $C > 0$, independent of h, such that

$$\|u-u_h^l\|_X+\|w-w_h^l\|_Y \leq C \inf_{(\eta_h,\xi_h)\in X_h\times Y_h} \|u-\eta_h^l\|_X+\|w-\xi_h^l\|_Y+h^k(\|f\|_{X^*}+\|g\|_{Y^*}).$$

Proof. For existence and uniqueness it is sufficient to prove existence for the homogeneous case $f_h = g_h = 0$ as the system is linear and finite dimensional. In the homogeneous case we see

$$c_h(u_h, u_h) + m_h(w_h, w_h) = 0.$$

We will denote by $G_h^l : Y^* \to X_h^l$ the map constructed in Lemma 5.2.1 and also define $G_h : Y^* \to X_h$ by $G_h := (l_h^X)^{-1} \circ G_h^l$. Notice also,

$$\begin{aligned}
\tilde{\beta}\|u_h^l - G_h^l m(w_h^l, \cdot)\|_X &\leq \sup_{\xi_h\in Y_h} \frac{b(u_h^l - G_h^l m(w_h^l, \cdot), \xi_h^l)}{\|\xi_h^l\|_Y},\\
&\leq \sup_{\xi_h\in Y_h} \frac{b(u_h^l, \xi_h^l) - b_h(u_h, \xi_h) + m_h(w_h, \xi_h) - m(w_h^l, \xi_h^l)}{\|\xi_h^l\|_Y},\\
&\leq Ch^k\|w_h^l\|_L.
\end{aligned}$$

The final line holds as $\|u_h^l\|_X \leq C\|w_h^l\|_L$ in the homogeneous case, using the second equation of the system. It follows, by (5.7),

$$\begin{aligned}
C\|w_h^l\|_L^2 &\leq c(G_h^l m(w_h^l, \cdot), G_h^l m(w_h^l, \cdot)) + m(w_h^l, w_h^l),\\
&= c(u_h^l, u_h^l) + m(w_h^l, w_h^l) - c_h(u_h, u_h) - m_h(w_h, w_h)\\
&\quad + c(G_h^l m(w_h^l, \cdot), G_h^l m(w_h^l, \cdot)) - c(u_h^l, u_h^l),\\
&\leq \tilde{C}h^k\|w_h^l\|_L^2.
\end{aligned}$$

Hence for h sufficiently small $w_h^l = 0$ from which we deduce $u_h^l = 0$ and hence $w_h = u_h = 0$. Thus there exists a unique solution for sufficiently small h. Now we prove the required error estimate. Let $\eta_h \in X_h$ and $\xi_h \in Y_h$ be arbitrary. Using the second equation and the discrete inf sup inequality it follows

$$
\begin{aligned}
\tilde{\beta}\|u_h^l-\eta_h^l\|_X &\le \sup_{v_h\in Y_h}\frac{1}{\|v_h^l\|_Y}\left[b(u_h^l-\eta_h^l,v_h^l)\right],\\
&= \sup_{v_h\in Y_h}\frac{1}{\|v_h^l\|_Y}\Big[b(u-\eta_h^l,v_h^l)-m(w-w_h^l,v_h^l)-\langle g,v_h^l\rangle+\langle g_h,v_h\rangle\\
&\qquad\qquad -b_h(u_h,v_h)+m_h(w_h,v_h)+b(u_h^l,v_h^l)-m(w_h^l,v_h^l)\Big],\\
&\le C\left[\|u-\eta_h^l\|_X+\|w-\xi_h^l\|_Y+\|w_h^l-\xi_h^l\|_L+h^k(\|g\|_{Y^*}+\|u_h^l\|_X+\|w_h^l\|_L)\right].
\end{aligned}
$$

We can produce a similar bound using the first equation of the system

$$
\begin{aligned}
\tilde{\gamma}\|w_h^l-\xi_h^l\|_Y &\le \sup_{v_h\in X_h}\frac{1}{\|v_h^l\|_X}\left[b(v_h^l,w_h^l-\xi_h^l)\right],\\
&= \sup_{v_h\in X_h}\frac{1}{\|v_h^l\|_X}\Big[b(v_h^l,w-\xi_h^l)+c(u-u_h^l,v_h^l)-\langle f,v_h^l\rangle+\langle f_h,v_h\rangle\\
&\qquad\qquad -b_h(v_h,w_h)-c_h(u_h,v_h)+b(v_h^l,w_h^l)+c(u_h^l,v_h^l)\Big],\\
&\le C\left[\|u-\eta_h^l\|_X+\|w-\xi_h^l\|_Y+\|u_h^l-\eta_h^l\|_X+h^k(\|f\|_{X^*}+\|u_h^l\|_X+\|w_h^l\|_Y)\right].
\end{aligned}
$$

Combining these two estimates produces the bound

$$
\begin{aligned}
\|u_h^l-\eta_h^l\|_X+\|w_h^l-\xi_h^l\|_Y \le C\Big[&\|u-\eta_h^l\|_X+\|w-\xi_h^l\|_Y+\|w_h^l-\xi_h^l\|_L\\
&+h^k(\|f\|_{X^*}+\|g\|_{Y^*}+\|u_h^l\|_X+\|w_h^l\|_Y)\Big].
\end{aligned}
\tag{5.11}
$$

To produce the result we must bound the L norm term which appears here. To do so we will add the discrete equations together and use the discrete coercivity relation (5.7). Firstly consider

$$
\begin{aligned}
&|c_h(u_h-\eta_h,u_h-\eta_h)+b_h(u_h-\eta_h,w_h-\xi_h)|\\
&=|c(u-\eta_h^l,u_h^l-\eta_h^l)+b(u_h^l-\eta_h^l,w-\xi_h^l)-\langle f,u_h^l-\eta_h^l\rangle+\langle f_h,u_h-\eta_h\rangle\\
&\quad +c(\eta_h^l,u_h^l-\eta_h^l)+b(u_h^l-\eta_h^l,\xi_h^l)-c_h(\eta_h,u_h-\eta_h)-b_h(u_h-\eta_h,\xi_h)|,\\
&\le C\|u_h^l-\eta_h^l\|_X\left[\|u-\eta_h^l\|_X+\|w-\xi_h^l\|_Y+h^k(\|f\|_{X^*}+\|\eta_h^l\|_X+\|\xi_h^l\|_Y)\right].
\end{aligned}
$$

Treating the second equation similarly produces

$$
\begin{aligned}
&|b_h(u_h-\eta_h,w_h-\xi_h)-m_h(w_h-\xi_h,w_h-\xi_h)|\\
&=|b(u-\eta_h^l,w_h^l-\xi_h^l)-m(w-\xi_h^l,w_h^l-\xi_h^l)-\langle g,w_h^l-\xi_h^l\rangle+\langle g_h,w_h-\xi_h\rangle\\
&\quad+b(\eta_h^l,w_h^l-\xi_h^l)-m(\xi_h^l,w_h^l-\xi_h^l)-b_h(\eta_h,w_h-\xi_h)+m_h(\xi_h,w_h-\xi_h)|,\\
&\le C\|w_h^l-\xi_h^l\|_Y\left[\|u-\eta_h^l\|_X+\|w-\xi_h^l\|_Y+h^k(\|g\|_{Y^*}+\|\eta_h^l\|_X+\|\xi_h^l\|_Y)\right].
\end{aligned}
$$

Combining these two estimates with (5.11) produces

$$
|c_h(u_h-\eta_h,u_h-\eta_h)+m_h(w_h-\xi_h,w_h-\xi_h)|\le C\left(\mathbb{B}^2+\mathbb{B}\|w_h^l-\xi_h^l\|_L\right), \tag{5.12}
$$

where the grouping of terms $\mathbb{B}$ is given by

$$
\begin{aligned}
\mathbb{B}:=&\|u-\eta_h^l\|_X+\|w-\xi_h^l\|_Y\\
&+h^k(\|f\|_{X^*}+\|g\|_{Y^*}+\|u_h^l\|_X+\|\eta_h^l\|_X+\|w_h^l\|_Y+\|\xi_h^l\|_Y).
\end{aligned} \tag{5.13}
$$

The coercivity relation in (5.7) gives

$$
C\|w_h^l-\xi_h^l\|_L^2\le c(G_h^l m(w_h^l-\xi_h^l,\cdot),G_h^l m(w_h^l-\xi_h^l,\cdot))+m(w_h^l-\xi_h^l,w_h^l-\xi_h^l),
$$

it follows

$$
\begin{aligned}
C\|w_h^l-\xi_h^l\|_L^2\le&|c(u_h^l-\eta_h^l,u_h^l-\eta_h^l)+m(w_h^l-\xi_h^l,w_h^l-\xi_h^l)\\
&-[c_h(u_h-\eta_h,u_h-\eta_h)+m_h(w_h-\xi_h,w_h-\xi_h)]\,|\\
&+|c_h(u_h-\eta_h,u_h-\eta_h)+m_h(w_h-\xi_h,w_h-\xi_h)|\\
&+|c(G_h^l m(w_h^l-\xi_h^l,\cdot),G_h^l m(w_h^l-\xi_h^l,\cdot))-c(u_h^l-\eta_h^l,u_h^l-\eta_h^l)|.
\end{aligned} \tag{5.14}
$$

To proceed we bound the three terms appearing here. The first term is simply an approximation property,

$$
\begin{aligned}
&|c(u_h^l-\eta_h^l,u_h^l-\eta_h^l)+m(w_h^l-\xi_h^l,w_h^l-\xi_h^l)-[c_h(u_h-\eta_h,u_h-\eta_h)+m_h(w_h-\xi_h,w_h-\xi_h)]\,|\\
&\le Ch^k\|u_h^l-\eta_h^l\|_X\left(\|u_h^l-\eta_h^l\|_X+\|w_h^l-\xi_h^l\|_Y\right),\\
&\le C\left(\mathbb{B}^2+\mathbb{B}\|w_h^l-\xi_h^l\|_L+h^k\|w_h^l-\xi_h^l\|_L^2\right).
\end{aligned} \tag{5.15}
$$

The final line is true for sufficiently small h and follows from (5.11). The second term we have already bounded in (5.12). For the final term notice

$$\begin{aligned}&|c(G_h^l m(w_h^l - \xi_h^l, \cdot), G_h^l m(w_h^l - \xi_h^l, \cdot)) - c(u_h^l - \eta_h^l, u_h^l - \eta_h^l)| \\ &\quad \leq C(\|G_h^l m(w_h^l - \xi_h^l, \cdot)\|_X + \|u_h^l - \eta_h^l\|_X)\|G_h^l m(w_h^l - \xi_h^l, \cdot) - (u_h^l - \eta_h^l)\|_X.\end{aligned}$$

To bound these terms first notice, by Lemma 5.2.1,

$$\|G_h^l m(w_h^l - \xi_h^l, \cdot)\|_X \leq C\|m(w_h^l - \xi_h^l, \cdot)\|_{Y^*} \leq C\|w_h^l - \xi_h^l\|_L.$$

We can then use the bound on $\|u_h^l - \eta_h^l\|_X$ established in (5.11) to produce

$$\begin{aligned}\|G_h^l m(w_h^l - \xi_h^l, \cdot)\|_X + \|u_h^l - \eta_h^l\|_X \leq \big[&\|u - \eta_h^l\|_X + \|w - \xi_h^l\|_Y + \|w_h^l - \xi_h^l\|_L \\ &+ h^k(\|f\|_{X^*} + \|g\|_{Y^*} + \|u_h^l\|_X + \|w_h^l\|_Y)\big].\end{aligned}$$

For the second factor we first use the triangle inequality to introduce $G_h(g_h^l)$, where $g_h^l \in (Y_h^l)^*$ is defined by

$$\langle g_h^l, v_h^l \rangle = \langle g_h, v_h \rangle.$$

Note that the map G_h^l is well defined on $(Y_h^l)^*$, see the proof of Lemma 5.2.1. By the triangle inequality

$$\|G_h^l m(w_h^l - \xi_h^l, \cdot) - (u_h^l - \eta_h^l)\|_X \leq \|G_h^l(m(w_h^l, \cdot) + g_h^l) - u_h^l\|_X + \|\eta_h^l - G_h^l(g_h^l + m(\xi_h^l, \cdot))\|_X.$$

To bound each of these we use the discrete inf sup inequalities and the definition of G_h. Firstly,

$$\begin{aligned}&\tilde{\beta}\|G_h^l(m(w_h^l, \cdot) + g_h^l) - u_h^l\|_X \leq \sup_{v_h \in Y_h} \frac{b(G_h^l(m(w_h^l, \cdot) + g_h^l) - u_h^l, v_h^l)}{\|v_h^l\|_Y}, \\ &= \sup_{v_h \in Y_h} \frac{1}{\|v_h^l\|_Y}\Big[-b(u_h^l, v_h^l) + b_h(u_h, v_h) - m_h(w_h, v_h) + m(w_h^l, v_h^l)\Big], \\ &\leq Ch^k\Big(\|u_h^l\|_X + \|w_h^l\|_Y\Big).\end{aligned}$$

Similarly for the second term

$$\begin{aligned}&\tilde{\beta}\|\eta_h^l - G_h^l(m(\xi_h^l, \cdot) + g_h^l)\|_X \leq \sup_{v_h \in Y_h} \frac{b(\eta_h^l - G_h^l(m(\xi_h^l, \cdot) + g_h^l), v_h^l)}{\|v_h^l\|_Y}, \\ &= \sup_{v_h \in Y_h} \frac{1}{\|v_h^l\|_Y}\Big[\langle g, v_h^l \rangle - \langle g_h, v_h \rangle + m(w - \xi_h^l, v_h^l) + b(\eta_h^l - u, v_h^l)\Big], \\ &\leq C(h^k\|g\|_{Y^*} + \|u - \eta_h^l\|_X + \|w - \xi_h^l\|_Y).\end{aligned}$$

Thus combining these bounds we see

$$|c(G_h^l m(w_h^l - \xi_h^l, \cdot), G_h^l m(w_h^l - \xi_h^l, \cdot)) - c(u_h^l - \eta_h^l, u_h^l - \eta_h^l)| \leq C\left(\mathbb{B}^2 + \mathbb{B}\|w_h^l - \xi_h^l\|_L\right). \tag{5.16}$$

Now, inserting (5.12), (5.15) and (5.16) into (5.14) and considering sufficiently small h, to absorb the final term appearing in (5.15) into the left hand side, produces

$$\|w_h^l - \xi_h^l\|_L^2 \leq C\left(\mathbb{B}^2 + \mathbb{B}\|w_h^l - \xi_h^l\|_L\right).$$

Thus by Young's inequality

$$\|w_h^l - \xi_h^l\|_L \leq C\mathbb{B}.$$

Inserting this bound into (5.11) gives

$$\begin{aligned}\|u_h^l - \eta_h^l\|_X + \|w_h^l - \xi_h^l\|_Y \leq C\Big[&\|u - \eta_h^l\|_X + \|w - \xi_h^l\|_Y + h^k(\|f\|_{X^*} + \|g\|_{Y^*}) \\ &+ h^k(\|u_h^l\|_X + \|\eta_h^l\|_X + \|w_h^l\|_Y + \|\xi_h^l\|_Y)\Big].\end{aligned}$$

We can deduce an a priori estimate by setting $\eta_h = \xi_h = 0$ as then

$$\|u_h^l\|_X + \|w_h^l\|_Y \leq C\left[\|u\|_X + \|w\|_Y + h^k(\|f\|_{X^*} + \|g\|_{Y^*} + \|u_h^l\|_X + \|w_h^l\|_Y)\right],$$

hence using the estimate in Theorem 5.2.2, for sufficiently small h,

$$\|u_h^l\|_X + \|w_h^l\|_Y \leq C\left[\|f\|_{X^*} + \|g\|_{Y^*}\right].$$

Using this bound and the triangle inequality gives

$$\begin{aligned}\|u - u_h^l\|_X + \|w - w_h^l\|_Y &\leq \|u - \eta_h^l\|_X + \|w - \xi_h^l\|_Y + \|u_h^l - \eta_h^l\|_X + \|w_h^l - \xi_h^l\|_Y \\ &\leq C\left[\|u - \eta_h^l\|_X + \|w - \xi_h^l\|_Y + h^k(\|f\|_{X^*} + \|g\|_{Y^*} + \|\eta_h^l\|_X + \|\xi_h^l\|_Y)\right].\end{aligned}$$

A further application of the triangle inequality and the a priori estimate in Theorem 5.2.2 produces

$$\begin{aligned}\|\eta_h^l\|_X + \|\xi_h^l\|_Y &\leq \|u - \eta_h^l\|_X + \|w - \xi_h^l\|_Y + \|u\|_X + \|w\|_Y, \\ &\leq \|u - \eta_h^l\|_X + \|w - \xi_h^l\|_Y + C(\|f\|_{X^*} + \|g\|_{Y^*}).\end{aligned}$$

Thus for sufficiently small h we have

$$\|u - u_h^l\|_X + \|w - w_h^l\|_Y \leq C \left[\|u - \eta_h^l\|_X + \|w - \xi_h^l\|_Y + h^k(\|f\|_{X^*} + \|g\|_{Y^*}) \right].$$

Now we obtain the required result by taking an infimum, as the left hand side is independent of ξ_h and η_h. □

This bound forms the core of the error analysis in our applications. There we will have the existence of an interpolation operator which allows this infimum bound to be turned into an error bound of the form Ch^α, for some $0 \leq \alpha \leq k$. Exactly how large this α can be depends upon the regularity of the solution (u, w). We now introduce this error bound in this abstract setting.

Corollary 5.4.1. *Suppose there exist Banach spaces $\tilde{X} \subset X$, $\tilde{Y} \subset Y$ such that $(u, w) \in \tilde{X} \times \tilde{Y}$ and with each embedding being continuous. Further assume there exists $\tilde{C}, \alpha > 0$, independent of h, such that*

$$\inf_{(\eta_h, \xi_h) \in X_h \times Y_h} \|u - \eta_h^l\|_X + \|w - \xi_h^l\|_Y \leq \tilde{C} h^\alpha \left(\|u\|_{\tilde{X}} + \|w\|_{\tilde{Y}} \right).$$

Then, for sufficiently small h, there exists $C > 0$, independent of h, such that

$$\|u - u_h^l\|_X + \|w - w_h^l\|_Y \leq C h^{\min\{\alpha, k\}} \left(\|u\|_{\tilde{X}} + \|w\|_{\tilde{Y}} + \|f\|_{X^*} + \|g\|_{Y^*} \right).$$

We can also establish higher order error bounds in weaker norms by using a duality argument similar to the Aubin-Nitsche trick. To do so we assume that $c(\cdot, \cdot)$ is symmetric and that the Banach spaces X and Y can be embedded into some larger Hilbert spaces which supply the appropriate weaker norms.

Proposition 5.4.1. *Under the assumptions of Corollary 5.4.1, further suppose $c(\cdot, \cdot)$ is symmetric and there exist Hilbert spaces H, J such that $X \subset H$ and $Y \subset J$ with both embeddings being continuous. Let $(\psi, \varphi) \in X \times Y$ denote the unique solution to Problem 5.2.1 with right hand side*

$$\eta \mapsto \langle u - u_h^l, \eta \rangle_H \quad \textit{and} \quad \xi \mapsto \langle w - w_h^l, \xi \rangle_J.$$

Assume that there exist Banach spaces $\hat{X} \subset X$ and $\hat{Y} \subset Y$ such that $(\psi, \varphi) \in \hat{X} \times \hat{Y}$ with both embeddings continuous and $\tilde{C}, \beta > 0$ such that

$$\inf_{(\eta_h, \xi_h) \in X_h \times Y_h} \|\psi - \eta_h^l\|_X + \|\varphi - \xi_h^l\|_Y \leq \tilde{C} h^\beta \left(\|\psi\|_{\hat{X}} + \|\varphi\|_{\hat{Y}} \right). \tag{5.17}$$

Finally assume the regularity result

$$\|\psi\|_{\hat{X}} + \|\varphi\|_{\hat{Y}} \leq \hat{C}(\|u - u_h^l\|_H + \|w - w_h^l\|_J). \tag{5.18}$$

Then, for sufficiently small h, there exists $C > 0$, independent of h, such that

$$\|u - u_h^l\|_H + \|w - w_h^l\|_J \leq Ch^{\min\{\alpha+\beta,k\}} \left(\|u\|_{\tilde{X}} + \|w\|_{\tilde{Y}} + \|f\|_{X^*} + \|g\|_{Y^*}\right).$$

Proof. Let (ψ, φ) be as defined in the statement above. It follows, for any $(\eta_h, \xi_h) \in X_h \times Y_h$,

$$\begin{aligned}
&\langle u - u_h^l, u - u_h^l \rangle_H + \langle w - w_h^l, w - w_h^l \rangle_J \\
=&c(u - u_h^l, \psi - \eta_h^l) + b(u - u_h^l, \varphi - \xi_h^l) + b(\psi - \eta_h^l, w - w_h^l) - m(w - w_h^l, \varphi - \xi_h^l) \\
&+ \langle f, \eta_h^l \rangle - \langle f_h, \eta_h \rangle + \langle g, \xi_h^l \rangle - \langle g_h, \xi_h \rangle - c(\eta_h^l, u_h^l) + c_h(\eta_h, u_h) \\
&- b(u_h^l, \xi_h^l) + b_h(u_h, \xi_h) - b(\eta_h^l, w_h^l) + b_h(\eta_h, w_h) + m(w_h^l, \eta_h^l) - m_h(\eta_h, w_h).
\end{aligned}$$

It follows, using the boundedness and approximation properties of the bilinear operators,

$$\begin{aligned}
&\langle u - u_h^l, u - u_h^l \rangle_H + \langle u - u_h^l, u - u_h^l \rangle_J \\
\leq& C\Big[(\|\psi - \eta_h^l\|_X + \|\varphi - \xi_h^l\|_Y)(\|u - u_h^l\|_X + \|w - w_h^l\|_Y) \\
&\quad + h^k(\|f\|_{X^*} + \|g\|_{Y^*})(\|\psi - \eta_h^l\|_X + \|\varphi - \xi_h^l\|_Y + \|\psi\|_X + \|\varphi\|_Y)\Big], \\
\leq& C(\|u - u_h^l\|_H + \|w - w_h^l\|_J) \left[h^{\min\{\alpha,k\}+\beta} \left(\|u\|_{\tilde{X}} + \|w\|_{\tilde{Y}}\right) + h^k \left(\|f\|_{X^*} + \|g\|_{Y^*}\right)\right].
\end{aligned}$$

The result is then deduced, for sufficiently small h, using Young's inequality. $\square$

5.5 Application of abstract finite element method

5.5.1 Clifford torus problems

We now apply the abstract finite element method in this context to produce a convergent finite element approximation for the Clifford torus problems.

Definition 5.5.1. *In the context of Definition 5.4.1, set $X_h = Y_h = \mathcal{S}_h$. Take l_h^X and l_h^Y to be the standard lift operator (see [27] for details). Set the bilinear* *functionals to be*

$$
\begin{aligned}
c_h(u_h, v_h) :=& \frac{1}{\rho}\sum_{k=1}^{K}\int_{\Gamma_h} u_h g_k^{-l}\, do_h \int_{\Gamma_h} v_h g_k^{-l}\, do_h + \chi_{con}\frac{1}{\delta}\sum_{k=1}^{N} u_h^l(X_k)v_h^l(X_k) \\
&+ \int_{\Gamma_h} \nabla_{\Gamma_h} u_h \cdot \left(\left[\frac{3}{2}H^2 - 2|\mathcal{H}|^2 - 2\right]\mathbb{1} - 2H\mathcal{H}\right)^{-l} \nabla_{\Gamma_h} v_h \\
&+ u_h v_h \left(-\frac{3}{2}H^2|\mathcal{H}|^2 + 2(\nabla_\Gamma\nabla_\Gamma H) : \mathcal{H} + |\nabla_\Gamma H|^2 + 2HTr(\mathcal{H}^3) + \Delta_\Gamma|\mathcal{H}|^2 + |\mathcal{H}|^4 - 1\right)^{-l} do_h, \\
b_h(u_h, v_h) :=& \int_{\Gamma_h} \nabla_{\Gamma_h} u_h \cdot \nabla_{\Gamma_h} v_h + u_h v_h \, do_h, \\
m_h(u_h, v_h) :=& \int_{\Gamma_h} u_h v_h \, do_h.
\end{aligned}
$$

Finally, set $g_h = 0$ *and* f_h *such that*

$$
\langle f_h, v_h\rangle = \sum_{k=1}^{N}\beta_k v_h^l(X_k) \quad \text{or} \quad \langle f_h, v_h\rangle = \frac{1}{\delta}\sum_{k=1}^{N}\alpha_k v_h^l(X_k).
$$

We shall check the assumptions made in Definition 5.4.1 hold in this context, we can then apply Theorem 5.4.1 to produce the following convergence result.

Corollary 5.5.1. *With the spaces and functionals chosen in Definition 5.3.1 and Definition 5.5.1, there exists* $h_0 > 0$ *such that for all* $0 < h < h_0$ *there exists a unique solution* $(u_h, w_h) \in X_h \times Y_h$ *to the problem*

$$
\begin{aligned}
c_h(u_h, \eta_h) + b_h(\eta_h, w_h) &= \langle f_h, \eta_h\rangle \quad \forall \eta_h \in X_h, \\
b_h(u_h, \xi_h) - m_h(w_h, \xi_h) &= \langle g_h, \xi_h\rangle \quad \forall \xi_h \in Y_h.
\end{aligned}
$$

Moreover there exists $C > 0$*, independent of* h*, such that*

$$
\|u - u_h^l\|_{1,2} + \|w - w_h^l\|_{0,2} \le Ch\|f\|_{X^*},
$$

for all $0 < h < h_0$.

Proof. Firstly, for the well posedness of the finite element method we need only check the assumptions made in Definition 5.4.1 hold for the choices made in Definition 5.5.1. The space $\mathcal{S}_h$ is a normed vector space and the standard lift operator is linear and injective, see [27] for details. Each of the functionals defined are bilinear by inspection and m_h is indeed symmetric.

The approximation properties for b_h, m_h and the H^1 type terms in c_h can be proven as in [27], in this case $k = 2$. Notice also we have treated c_h analogously to the treatment of the diffusion term in [26]. For the remaining terms in c_h, the $1/\rho$ term can be treated in the same manner as the L^2 inner product and for the $1/\delta$ term observe that no contribution to the approximation error is made. A similar observation shows, in this case,

$$\langle f_h, v_h \rangle = \langle f, v_h^l \rangle.$$

Hence f_h satisfies the required approximation property as does g_h because $g_h = g = 0$. We thus have satisfied all of the assumptions of Definition 5.4.1, hence the discrete problem is well posed by Theorem 5.4.1. For the convergence result we will argue as in Proposition 5.4.1, however the dual problem gains no further regularity in this circumstance so a more careful argument is required. Let $(\psi, \varphi) \in X \times Y$ denote the solution to Problem 5.2.1 with right hand side

$$\eta \mapsto \langle u - u_h^l, \eta \rangle_{H^1(\Gamma)} \quad \text{and} \quad \xi \mapsto \langle w - w_h^l, \xi \rangle_{L^2(\Gamma)}.$$

It follows

$$\begin{aligned} &\|u - u_h^l\|_{1,2}^2 + \|w - w_h^l\|_{0,2}^2 \\ &\qquad = c(\psi, u - u_h^l) + b(u - u_h^l, \varphi) + b(\psi, w - w_h^l) - m(\varphi, w - w_h^l). \end{aligned}$$

As $g = g_h = 0$ in this case it follows

$$b(u, \varphi) - m(\varphi, w) = 0.$$

Furthermore,

$$b(u_h^l, \varphi) = b(u_h^l, \Pi_h \varphi) - b_h(u_h, \Pi_h^{-l} \varphi) + m_h(w_h, \Pi_h^{-l} \varphi),$$

hence

$$\begin{aligned} |b(u - u_h^l, \varphi) - m(w - w_h^l, \varphi)| &\leq |m(w_h^l, \varphi - \Pi_h \varphi)| + Ch^2(\|u_h^l\|_X + \|w_h^l\|_Y)\|\varphi\|_Y \\ &\leq \|w_h^l\|_{0,2}\|\varphi - \Pi_h \varphi\|_{0,2} + Ch^2\|f\|_{X^*}\|w - w_h^l\|_{0,2} \\ &\leq Ch\|f\|_{X^*}\|w - w_h^l\|_{0,2}. \end{aligned}$$

The final line follows from the bound shown in (5.10). To deal with the two remaining terms observe, for any $\eta_h \in \mathcal{S}_h$,

$$|c(\eta_h^l, u - u_h^l) + b(\eta_h^l, w - w_h^l)| \leq |\langle f, \eta_h^l \rangle - \langle f_h \eta_h \rangle| + Ch^2\|\eta_h^l\|_X(\|u_h^l\|_X + \|w_h^l\|_Y),$$

where the Ch^2 terms are produced by geometric estimates in the usual manner. Setting $\eta_h^l = I_h^l \psi$, the Lagrange interpolant, we obtain

$$
\begin{aligned}
&|c(\psi, u - u_h^l) + b(\psi, w - w_h^l)| \\
&\leq |c(\psi - I_h^l \psi, u - u_h^l) + b(\psi - I_h^l \psi, w - w_h^l)| + Ch^2 \|\psi\|_X \|f\|_{X^*} \\
&\leq Ch \|u - u_h^l\|_{1,2} \|f\|_{X^*}.
\end{aligned}
$$

The result then follows by combining the estimates derived above. □

5.5.2 General fourth order problem

We now consider the general fourth order problem and use the abstract theory to produce a convergent finite element method. We will again use P^1 finite elements, in this case we will achieve optimal error bounds for both u and w of order h convergence in the H^1 norm and order h^2 in the L^2 norm.

Definition 5.5.2. *In the context of Definition 5.4.1, set $X_h = Y_h = \mathcal{S}_h$. Take l_h^X and l_h^Y to be the standard lift operator (see [27] for details). Set the bilinear functionals to be*

$$
\begin{aligned}
c_h(u_h, v_h) &:= \int_{\Gamma_h} (\mathcal{B}^{-l} - 2\mathbb{1}) \nabla_{\Gamma_h} u_h \cdot \nabla_{\Gamma_h} v_h + \left(\mathcal{C}^{-l} - 1 \right) u_h v_h \, do_h, \\
b_h(u_h, v_h) &:= \int_{\Gamma_h} \nabla_{\Gamma_h} u_h \cdot \nabla_{\Gamma_h} v_h + u_h v_h \, do_h, \\
m_h(u_h, v_h) &:= \int_{\Gamma_h} u_h v_h \, do_h.
\end{aligned}
$$

Finally, set

$$
f_h := m_h(\mathcal{F}^{-l}, \cdot) \quad \text{and} \quad g_h := m_h(\mathcal{G}^{-l}, \cdot).
$$

We can now prove convergence for this method, in this example we have more regularity than the problems involving a delta function meaning we recover the optimal orders of convergence for P^1 elements.

Corollary 5.5.2. *With the spaces and functionals chosen in Definition 5.3.2 and Definition 5.5.2, there exists $h_0 > 0$ such that for all $0 < h < h_0$ there exists a unique solution $(u_h, w_h) \in X_h \times Y_h$ to the problem*

$$
\begin{aligned}
c_h(u_h, \eta_h) + b_h(\eta_h, w_h) &= \langle f_h, \eta_h \rangle \quad \forall \eta_h \in X_h, \\
b_h(u_h, \xi_h) - m_h(w_h, \xi_h) &= \langle g_h, \xi_h \rangle \quad \forall \xi_h \in Y_h.
\end{aligned}
$$

Moreover there exists $C > 0$, independent of h, such that

$$\|u - u_h^l\|_{i,2} + \|w - w_h^l\|_{i,2} \leq Ch^{2-i}(\|\mathcal{F}\|_{0,2} + \|\mathcal{G}\|_{0,2}),$$

for each $i = 0, 1$ and for all $0 < h < h_0$.

Proof. For the $i = 1$ case we apply Corollary 5.4.1, the assumptions on the lift operators and bilinear functionals made in Definition 5.4.1 hold by the same arguments as for the Clifford torus application. For the approximation to the data follow the proof of Lemma 4.7 in [27],

$$|m(\mathcal{F}, \eta_h^l) - m_h(\mathcal{F}^{-l}, \eta_h)| \leq Ch^2 |m(\mathcal{F}, \eta_h^l)| \leq Ch^2 \|m(\mathcal{F}, \cdot)\|_{X^*} \|\eta_h^l\|_X,$$

an identical argument holds for $\mathcal{G}$. Set the spaces $\tilde{X} = \tilde{Y} = H^2(\Gamma)$ and $\alpha = 1$, the approximation assumption in Corollary 5.4.1 holds by the standard interpolation estimates (see e.g. [27, Lemma 4.3]). It follows

$$\|u - u_h^l\|_{1,2} + \|w - w_h^l\|_{1,2} \leq Ch\left(\|u\|_{2,2} + \|w\|_{2,2} + \|m(\mathcal{F}, \cdot)\|_{-1,2} + \|m(\mathcal{G}, \cdot)\|_{-1,2}\right).$$

Hence by the regularity estimate in Proposition 5.3.2 and the continuous embedding $H^1(\Gamma) \subset L^2(\Gamma)$ we have

$$\|u - u_h^l\|_{1,2} + \|w - w_h^l\|_{1,2} \leq Ch\left(\|\mathcal{F}\|_{0,2} + \|\mathcal{G}\|_{0,2}\right).$$

For the $i = 0$ result we use Proposition 5.4.1, setting $H = J = L^2(\Gamma)$ and $\hat{X} = \hat{Y} = H^2(\Gamma)$. The approximation condition (5.17) holds for $\beta = 1$ by the standard interpolation estimates. The regularity result (5.18) holds by elliptic regularity applied to the dual problem. It follows

$$\|u - u_h^l\|_{0,2} + \|w - w_h^l\|_{0,2} \leq Ch^2\left(\|\mathcal{F}\|_{0,2} + \|\mathcal{G}\|_{0,2}\right).$$

□

5.6 Numerical examples

We conclude with numerical examples showing that these theoretical convergence rates are achieved in practice. All of the numerical examples given here have been implemented in the DUNE framework [5, 6, 9], making particular use of the DUNE-FEM module [19].

5.6.1 Lower regularity problem

We will first study a problem similar to the point forces problem introduced in Definition 5.3.1. For ease of construction of an exact solution we will not study this problem precisely but a similar one whose solution exhibits the same regularity, $(u, w) \in W^{3,p}(\Gamma) \times W^{1,p}(\Gamma)$ for any $1 < p < 2$, as proven in Corollary 5.3.1. Note that this is the limiting regularity result, it is not true for $p = 2$. To construct such a problem take Γ to be the unit sphere, $\Gamma = S(0, 1)$ and consider the function

$$w(x) = -\frac{1}{4\pi}\left[\log(1 - x_3) - \log(2) + 1 + 3x_3\right].$$

The function has a smooth part and a logarithmic part which is based upon the Green's function for the Laplace Beltrami operator on a sphere, see [49]. That is, in a distributional sense, w satisfies

$$-\Delta_\Gamma w = \delta_N - \frac{1}{4\pi} - \frac{3}{4\pi}x_3,$$

where δ_N is a delta function centred at the north pole $N = (0, 0, 1)$. The logarithmic part of w lies in $W^{1,p}(\Gamma)$ for any $1 < p < 2$ but is not in $H^1(\Gamma)$. We take u to be

$$u(x) = \frac{1}{8\pi}\left[(1 - x_3)\log(1 - x_3) + \frac{1}{2} - \log(2)\right].$$

The resulting coupled problem we study, in distributional form, is given by

$$\begin{aligned}\Delta_\Gamma u + 2u - \Delta_\Gamma w + w &= \delta_N - \frac{1}{4\pi} - \frac{3}{4\pi}x_3\\ -\Delta_\Gamma u + u - w &= \frac{3}{8\pi}\left[(1 - x_3)\log(1 - x_3) + \frac{1}{2} - \log(2)\right]\end{aligned}$$

This can be viewed as a splitting method which solves the fourth order PDE

$$\begin{aligned}\Delta_\Gamma^2 u - \Delta_\Gamma u + 3u =& \delta_N - \frac{1}{4\pi} - \frac{3}{4\pi}x_3 + \frac{3}{8\pi}\left[(1 - x_3)\log(1 - x_3) + \frac{1}{2} - \log(2)\right]\\ &+ \frac{3}{8\pi}\left[(1 - x_3)\log(1 - x_3) + \frac{1}{2} - \log(2)\right].\end{aligned}$$

The weak formulation and discretisation of the system is completely analogous to the treatment of the point forces problem described in Definition 5.3.1 and Definition 5.5.1. Explicitly, in terms of the general abstract formulation in Problem 5.2.1, we choose

$$\begin{aligned}
c(u,v) &:= \int_\Gamma -\nabla_\Gamma u \cdot \nabla_\Gamma v + 2uv \; do, \\
b(u,w) &:= \int_\Gamma \nabla_\Gamma u \cdot \nabla_\Gamma v + uv \; do, \\
m(u,v) &:= \int_\Gamma uv \; do, \\
\langle f, v \rangle &:= v(0,0,1) - \frac{1}{4\pi} \int_\Gamma v \; do - \frac{3}{\pi} \int_\Gamma x_3 v \; do, \\
\langle g, v \rangle &:= \int_\Gamma \frac{3}{8\pi} \left[(1-x_3)\log(1-x_3) + \frac{1}{2} - \log(2) \right] v \; do.
\end{aligned}$$

The finite element method formulation is also completely analogous to the treatment of the point forces problem. Explicitly, in terms of the general abstract formulation in Problem 5.4.1, we choose

$$\begin{aligned}
c_h(u_h,v_h) &:= \int_{\Gamma_h} -\nabla_{\Gamma_h} u_h \cdot \nabla_{\Gamma_h} v_h + 2u_h v_h \; do_h, \\
b_h(u_h,w_h) &:= \int_{\Gamma_h} \nabla_{\Gamma_h} u_h \cdot \nabla_{\Gamma_h} v_h + u_h v_h \; do_h, \\
m_h(u_h,v_h) &:= \int_{\Gamma_h} u_h v_h \; do_h, \\
\langle f_h, v_h \rangle &:= v_h(p^{-1}(0,0,1)) - \frac{1}{4\pi} \int_{\Gamma_h} v_h \; do - \frac{3}{\pi} \int_{\Gamma_h} (x_3)^{-l} v_h \; do_h, \\
\langle g_h, v_h \rangle &:= \int_{\Gamma_h} \frac{3}{8\pi} \left[(1-x_3)\log(1-x_3) + \frac{1}{2} - \log(2) \right]^{-l} v_h \; do_h.
\end{aligned}$$

Similarly, the finite element method converges at the rates proven in Corollary 5.5.1, we can compare this to the experimental order of convergence obtained in practice. The results are given in Table 5.1 and Table 5.2. In each case, for grid size h, $E_V(h)$ is the error in the V norm of the finite element approximation. For example in Table 5.1 we have

$$E_{L^2(\Gamma)}(h) := \|u - u_h^l\|_{0,2}.$$

The experimental order of convergence (EOC) with respect to the V-norm, for tests with grid sizes h_1 and h_2, is given by

$$EOC = \frac{\log(E_V(h_1)/E_V(h_2))}{\log(h_1/h_2)}.$$

In each of our examples the EOC is calculated between the current h and the previous refinement, so that the denominator is $\log(1/2)$ each time as the mesh size halves with each refinement.

h	$E_{L^2(\Gamma)}(h)$	EOC	$E_{H^1(\Gamma)}(h)$	EOC
1.41421	7.2206×10^{-2}	-	9.60127×10^{-2}	-
7.07106×10^{-1}	2.68314×10^{-2}	1.4282	4.81314×10^{-2}	0.996248
3.53553×10^{-1}	7.71427×10^{-3}	1.79832	2.4304×10^{-2}	0.985781
1.76776×10^{-1}	2.04304×10^{-3}	1.91681	1.24533×10^{-2}	0.964672
8.83883×10^{-2}	5.30802×10^{-4}	1.94447	6.31331×10^{-3}	0.980055
4.41941×10^{-2}	1.37634×10^{-4}	1.94734	3.17379×10^{-3}	0.992192
2.20970×10^{-2}	3.57961×10^{-5}	1.94296	1.58979×10^{-3}	0.997373
1.10485×10^{-2}	9.3513×10^{-6}	1.93656	7.95344×10^{-4}	0.999182
5.52427×10^{-3}	2.45312×10^{-5}	1.93055	3.97739×10^{-4}	0.999757

Table 5.1: Errors and Experimental orders of convergence for $u_h^l - u$.

h	$E_{L^2(\Gamma)}(h)$	EOC
1.41421	1.28739×10^{-1}	-
7.07106×10^{-1}	4.91831×10^{-2}	1.38821
3.53553×10^{-1}	2.37553×10^{-2}	1.04991
1.76776×10^{-1}	1.25937×10^{-2}	0.915547
8.83883×10^{-2}	6.5736×10^{-3}	0.937948
4.41941×10^{-2}	3.35583×10^{-3}	0.970015
2.20970×10^{-2}	1.69215×10^{-3}	0.987811
1.10485×10^{-2}	8.48703×10^{-4}	0.995527
5.52427×10^{-3}	4.24803×10^{-4}	0.998466

Table 5.2: Errors and Experimental orders of convergence for $w_h^l - w$.

The experimental orders of convergence observed are consistent with the bounds proven theoretically, order h convergence for $\|u - u_h^l\|_{1,2}$ and $\|w - w_h^l\|_{0,2}$, indicating that these bounds are optimal. We have also tested the L^2 error for $u - u_h^l$. The results are consistent with an error of order $h^2|\log h|$ as was observed in the decoupled problem over a sphere. As such we may conjecture that this is indeed the order of convergence in this weaker norm but have no rigorous proof at this time.

5.6.2 Higher regularity problem

We consider the problem outlined in Definition 5.3.2, setting $\Gamma = S(0,1)$, the unit sphere, taking

$$\mathcal{B}(x) = \begin{pmatrix} x_1 & 0 & 0 \\ 0 & x_2 & 0 \\ 0 & 0 & x_3 \end{pmatrix}, \; \mathcal{C}(x) = 2 + x_1x_2, \; C_m = 3/2, \; C_M = 5/2, \; \lambda_M = 1, \; \Lambda = 1$$

and selecting

$$\begin{aligned}\mathcal{F}(x) :=& -5x_3(x_1^3 + x_2^3 + x_3^3) + 2x_3(x_1 + x_2 + x_3) - 4x_3 + 4x_3^2 - 1 + (1 + x_1x_2)x_3 + 7x_1x_2, \\ \mathcal{G}(x) :=& 3x_3 - x_1x_2.\end{aligned}$$

These choices for $\mathcal{F}$ and $\mathcal{G}$ give the solution $(u, w) = (\nu_3, \nu_1\nu_2)$. The example is chosen as it shows that this method can be used to split a fourth order problem where the second order terms make an indefinite contribution to the bilinear form. Explicitly, the fourth order equation solved by u is

$$\Delta_\Gamma^2 u - \nabla_\Gamma \cdot (\mathcal{B}\nabla_\Gamma u) + 2\mathcal{B}\nabla_\Gamma u \cdot \nu + \mathcal{C}u = \mathcal{F} + \Delta_\Gamma \mathcal{G} - \mathcal{G}.$$

The resulting errors and experimental orders of convergence are shown below.

h_n	$E_{L^2(\Gamma)}(h_n)$	EOC	$E_{H^1(\Gamma)}(h_n)$	EOC
1.41421	5.50789×10^{-1}	-	9.56541×10^{-1}	-
7.07106×10^{-1}	1.87047×10^{-1}	1.5581	5.93089×10^{-1}	0.689579
3.53553×10^{-1}	5.03273×10^{-2}	1.89399	3.11093×10^{-1}	0.930903
1.76776×10^{-1}	1.29141×10^{-2}	1.96239	1.57072×10^{-1}	0.985921
8.83883×10^{-2}	3.25813×10^{-3}	1.98683	7.88294×10^{-2}	0.994618
4.41941×10^{-2}	8.17079×10^{-4}	1.9955	3.94719×10^{-2}	0.997907
2.20970×10^{-2}	2.04483×10^{-4}	1.99849	1.97459×10^{-2}	0.999277
1.10485×10^{-2}	5.11382×10^{-5}	1.99951	9.87451×10^{-3}	0.999769
5.52427×10^{-3}	1.27861×10^{-5}	1.99983	4.9375×10^{-3}	0.99993

Table 5.3: Errors and Experimental orders of convergence for $u_h^l - u$.

Observe that the method achieves the orders of convergence proven in Corollary 5.5.2, order h and h^2 convergence in the H^1 and L^2 norms respectively.

h_n	$E_{L^2(\Gamma)}(h_n)$	EOC	$E_{H^1(\Gamma)}(h_n)$	EOC
1.41421	8.2062×10^{-1}	-	2.06098	-
7.07106×10^{-1}	5.04944×10^{-1}	0.689579	1.31633	0.646807
3.53553×10^{-1}	1.75493×10^{-1}	1.52471	6.67723×10^{-1}	0.9792
1.76776×10^{-1}	4.78556×10^{-2}	1.87466	3.25700×10^{-1}	1.03571
8.83883×10^{-2}	1.22409×10^{-2}	1.96698	1.61395×10^{-1}	1.01295
4.41941×10^{-2}	3.07844×10^{-3}	1.99143	8.05016×10^{-2}	1.0035
2.20970×10^{-2}	7.70788×10^{-4}	1.99779	4.02261×10^{-2}	1.00088
1.10485×10^{-2}	1.92773×10^{-4}	1.99943	2.01100×10^{-2}	1.00022
5.52427×10^{-3}	4.81981×10^{-5}	1.99985	1.00546×10^{-1}	1.00005

Table 5.4: Errors and Experimental orders of convergence for $w_h^l - w$.

Appendix A

Abstract minimisation problems

A.1 Abstract quadratic programming problem

We begin by introducing a general Hilbert space quadratic programming problem (QPP). This general framework allows us to develop abstract results that can be applied to a variety of the problems which result from modelling membranes.

Definition A.1.1 (Quadratic programming problem (QPP)).
Let V be a Hilbert Space, fix $N \in \mathbb{N} \setminus \{0\}$, $\alpha \in \mathbb{R}^N$ and a set of linearly independent functionals $\{F_1, ..., F_N\} \subset V^*$. We thus define a convex subset $K_\alpha^F \subset V$ by

$$K_\alpha^F := \{v \in V \mid F_j(v) = \alpha_j \;\forall\, 1 \leq j \leq N\}.$$

Let $a : V \times V \to \mathbb{R}$ be a bilinear, symmetric, bounded and coercive functional.
Let $l : V \to \mathbb{R}$ be a bounded linear functional.
Define $J : V \to \mathbb{R}$ by $J(v) := \frac{1}{2}a(v, v) - l(v)$.
We will say $u \in K_\alpha^F$ is a minimiser of J over K_α^F if $J(u) \leq J(v) \;\forall\, v \in K_\alpha^F$.

In the above we have the superscript $F := (F_1, ..., F_N)$ denoting that the convex set depends upon our choice of the linear functionals. We will show the existence and uniqueness of such a minimiser and begin with a standard lemma relating the minimisation problem to two variational problems.

Lemma A.1.1 (Equivalent variational problems).
Using the notions in Definition A.1.1, suppose $u \in K_\alpha^F$, then the following are equivalent:

1. $J(u) \leq J(v) \;\; \forall v \in K_\alpha^F$.

2. $a(u, v - u) \geq l(v - u) \;\; \forall v \in K_\alpha^F$.

3. $a(u,w) = l(w)\ \ \forall w \in K_0^F$.

Proof. (1) $\iff$ (2) :
Notice J is convex and Gateaux differentiable over V. The Gateaux derivative at any $v \in V$ is given by $J'(v) = a(v,\cdot) - l(\cdot)$. The equivalence is then a standard result in convex optimization.
(2) $\iff$ (3) :
Suppose (3), for any $v \in K_\alpha^F$ we have $v - u \in K_0^F$ hence $a(u, v-u) = l(v-u) \geq l(v-u)$.
Suppose (2), for any $w \in K_0^F$ we have $w+u \in K_\alpha^F$ hence $a(u,w) = a(u,(w+u)-u) \geq l(w)$. By applying this to $-w$ also we obtain the required equality. $\square$

We now construct $u \in K_\alpha^F$ that satisfies the third condition above and hence is a minimiser, first we fix some notation.

Definition A.1.2 (Basis functions)**.**
Using the notions in Definition A.1.1, for each $1 \leq j \leq N$ *define* $\phi_j \in V$ *by the unique solution to*

$$a(\phi_j, v) = F_j(v)\ \forall\, v \in V.$$

Hence define the matrix $A = (a_{ij})_{i,j=1,\ldots,N}$ *by* $a_{ij} := a(\phi_i, \phi_j)$.
Finally, define $\phi_0 \in K_0^F$ *by the unique solution to*

$$a(\phi_0, v) = l(v)\ \forall\, v \in K_0^F.$$

Notice A is symmetric and invertible as it is defined by a symmetric, coercive bilinear functional applied to linearly independent elements of V.

Proposition A.1.1 (Existence and uniqueness of minimiser)**.**
There exists a unique $u \in K_\alpha^F$ *such that* $J(u) \leq J(v)\ \forall\, v \in K_\alpha^F$, *moreover* $u \in Sp\,\{\phi_0, ..., \phi_N\}$.

Proof. Define $\lambda \in \mathbb{R}^N$ by $\lambda := A^{-1}\alpha$ and thus define $u^* \in V$ by

$$u^* := \phi_0 + \sum_{j=1}^{N} \lambda_j \phi_j.$$

Notice $u^* \in K_\alpha^F$, as for any $1 \leq i \leq N$ we have

$$F_i(u^*) = F_i(\phi_0) + \sum_{j=1}^{N} \lambda_j F_i(\phi_j) = (A\lambda)_i = \alpha_i.$$

Now let $w \in K_0^F$, then

$$a(u^*, w) = a(\phi_0, w) + \sum_{j=1}^{N} \lambda_j a(\phi_j, w) = l(w) + \sum_{j=1}^{N} \lambda_j F_j(w) = l(w).$$

Thus $u^* \in K_\alpha^F$ satisfies the equivalent variational problem, so it is a minimiser of J over K_α^F.
For uniqueness, suppose $v \in K_\alpha^F$ is also a minimiser of J over K_α^F. Thus $u^* - v \in K_0^F$ and

$$a(u^* - v, u^* - v) = a(u^*, u^* - v) - a(v, u^* - v) = l(u^* - v) - l(u^* - v) = 0.$$

By coercivity of a we have $v = u^*$. $\square$

In the above we have minimised the energy functional J over a convex set which accounts for the constraints applied by the linear functionals F_i. We now wish to obtain a global minimiser by allowing the functionals to vary over some subset $\mathscr{G} \subset (V^*)^N$.

Definition A.1.3 (QPP global minimisers)**.**
In the setting of Definition A.1.1, let $\mathscr{G} \subset (V^*)^N$. We thus define $L_\alpha \subset V$ by

$$L_\alpha := \{v \in V \mid \exists G = (G_1, ..., G_N) \in \mathscr{G} \text{ s.t. } G_i(v) = \alpha_i \; \forall 1 \leq i \leq N\}.$$

We will say $u \in L_\alpha$ is a QPP global minimiser if $J(u) \leq J(v) \; \forall v \in L_\alpha$.

We will show existence of these global minimisers shortly. We first require a slight generalisation of the QPP by relaxing the condition that the linear functionals $F_1, ..., F_N$ must be linearly independent. This is done in the following lemma.

Lemma A.1.2 (Generalised QPP)**.**
In the setting of Definition A.1.1. Let $\{F_1, ..., F_N\} \subset V^*$ be an arbitrary subset and define K_α^F as previously. Then we have the following equivalence

$$\exists!\, u \in K_\alpha^F \text{ s.t. } J(u) \leq J(v) \; \forall v \in K_\alpha^F \iff K_\alpha^F \neq \emptyset.$$

Proof. The forwards implication is trivial, we prove the backwards implication by induction on N. Base Case, $N = 1$:
For $N = 1$ we have two cases to consider. Firstly, if $F_1 = 0$ we must have $\alpha_1 = 0$, else K_α^F would be empty. Now we have $K_\alpha^F = V$ and the existence and uniqueness of a minimiser over V is a standard result, it is equivalent to the existence of a unique

solution in V to the variational problem $a(u,v) = l(v)\ \forall v \in V$. The remaining case is that $F_1 \neq 0$, then $\{F_1\}$ is linearly independent and we have a unique minimiser over K_α^F by Proposition A.1.1.

For the inductive hypothesis suppose the backwards implication holds for some $N \geq 1$. For $N+1$ we have two cases to consider. Firstly, if $\{F_1, ..., F_{N+1}\}$ is linearly independent we have a unique minimiser over K_α^F by Proposition A.1.1. Now assume $\{F_1, ..., F_{N+1}\}$ is linearly dependent. Without loss of generality we may then write $F_{N+1} = \sum_{j=1}^N \lambda_j F_j$. As $K_\alpha^F \neq \emptyset$ find $v \in K_\alpha^F$, then

$$\alpha_{N+1} = F_{N+1}(v) = \sum_{j=1}^N \lambda_j F_j(v) = \sum_{j=1}^N \lambda_j \alpha_j.$$

Hence $K_\beta^G = K_\alpha^F$, where $G = (F_1, ..., F_N)$ and $\beta = (\alpha_1, ..., \alpha_N)$. We thus have an N-dimensional problem, which has a unique minimiser by the inductive hypothesis. $\square$

We will write u_F to denote the unique minimiser of J over K_α^F when $K_\alpha^F \neq \emptyset$. We may now prove the existence of QPP global minimisers.

Proposition A.1.2 (Existence of QPP global minimisers)**.**
Using the notions in Definition A.1.3, suppose $\mathscr{G} \subset (V^*)^N$ is compact and that $L_\alpha \neq \emptyset$ then there exists a QPP global minimiser.

Proof. Define a map $\xi : \mathscr{G} \to \mathbb{R}$ by

$$\xi(G) := \begin{cases} J(u_G) & \text{if } K_\alpha^G \neq \emptyset, \\ \infty & \text{otherwise.} \end{cases}$$

By assumption $L_\alpha \neq \emptyset$ and thus there exists $G \in \mathscr{G}$ such that $K_\alpha^G \neq \emptyset$. Hence ξ does take finite values for some $G \in \mathscr{G}$. Furthermore, whenever G is such that $K_\alpha^G \neq \emptyset$ we have

$$\xi(G) = \frac{1}{2}a(u_G, u_G) - l(u_G) \geq \frac{1}{2}C_c\|u_G\|_V^2 - C_l\|u_G\|_V \geq -\frac{C_l^2}{2C_c}.$$

Thus define $m := \inf_{G\in\mathscr{G}} \xi(G)$ and by the above m is finite. By the approximation property we may find a sequence $(G^n)_{n=1}^\infty \subset \mathscr{G}$ such that $m \leq \xi(G^n) < m + 1/n$. As $\xi(G^n) < m + 1\ \forall n \geq 1$ then in fact $K_\alpha^{G^n} \neq \emptyset$ for each n and thus $\xi(G^n) = J(u_{G^n})$. In what follows we will use many results that involve taking a subsequence, we will assume in each case that we have already chosen the correct sequence.

As $\mathscr{G}$ is compact we may assume $G^n \to G$ for some $G \in \mathscr{G}$. Furthermore, for each

$n \geq 1$ it holds

$$\frac{1}{2} C_c \|u_{G^n}\|_V^2 - C_l \|u_{G^n}\|_V \leq J(u_{G^n}) < m + 1 \implies \|u_{G^n}\|_V \leq B.$$

The bound $B > 0$ is independent of n, it depends only upon C_c, C_l and m. We may thus assume $u_n := u_{G^n} \rightharpoonup u$, some $u \in V$. We may also assume $\|u_n\|_V$ is convergent (in the sense of real sequences) and by the weak lower semi-continuity of Hilbert space norms we have that

$$\|u\|_V \leq \liminf_{n\to\infty} \|u_n\|_V = \lim_{n\to\infty} \|u_n\|_V.$$

It then follows

$$J(u) \leq \liminf_{n\to\infty} J(u_n) = \lim_{n\to\infty} \frac{1}{2}\|u_n\|_V^2 - l(u_n) \leq \lim_{n\to\infty} m + 1/n = m.$$

Notice, for each $1 \leq i \leq N$ we have

$$G_i(u) = \lim_{n\to\infty} G_i^n(u_n) = \lim_{n\to\infty} \alpha_i = \alpha_i.$$

thus $u \in K_\alpha^G$. We then have $K_\alpha^G \neq \emptyset$ and we may find u_G minimising J over K_α^G. We then have $m \leq J(u_G) \leq J(u) \leq m$ so we have equality and by uniqueness $u = u_G$. We have thus constructed a QPP global minimiser as for any $v \in L_\alpha$, $v \in K_\alpha^F \neq \emptyset$ for some $F \in \mathscr{G}$, then

$$J(v) \geq J(u_F) \geq m = J(u_G).$$

We now only need that $u_G \in L_\alpha$, this is immediate from $u \in K_\alpha^G$. $\square$

Having proven the existence of QPP global minimisers we now produce an equivalent condition for minimisers which will prove useful for the applications. This is similar to a result in [12] which studies a similar problem. Note that the additional assumption, that u a QPP global minimiser implies $u \in K_\alpha^G$ for some $G \in \tilde{\mathscr{G}}$, will follow essentially without loss of generality in our applications.

Lemma A.1.3 (Equivalent condition for QPP global minimiser).
Using the notions in Proposition A.1.1, let $w \in V$ be the unique solution to

$$a(w, v) = l(v) \; \forall v \in V.$$

Define $\tilde{\mathscr{G}} := \{G = (G_1, ..., G_N) \in \mathscr{G} \mid G_1, ..., G_N$ are linearly independent$\}$. Suppose our problem is such that u a QPP global minimiser implies $u \in K_\alpha^G$ for some $G \in \tilde{\mathscr{G}}$. For $G \in \tilde{\mathscr{G}}$ define the matrix $A_G \in \mathbb{R}^{N\times N}$ by $(A_G)_{ij} = a(\phi_i, \phi_j)$. Here the ϕ_i are

the basis functions defined previously, notice that these depend on G. Finally, define $G(w) \in \mathbb{R}^N$ by $G(w) := (G_1(w), G_2(w), ..., G_N(w))$.
Then there exists $F \in \tilde{\mathscr{G}}$ s.t.

$$(A_F)^{-1}(\alpha - F(w)) \cdot (\alpha - F(w)) = \inf_{G \in \tilde{\mathscr{G}}} (A_G)^{-1}(\alpha - G(w)) \cdot (\alpha - G(w)).$$

Furthermore u is a QPP global minimiser if and only if $u = w + \psi_{F'}$ where $F' \in \tilde{\mathscr{G}}$ achieves the minimum of the function above and $\psi_{F'}$ is the unique minimiser of $v \mapsto \frac{1}{2}a(v,v)$ over $K^{F'}_{(\alpha - F'(w))}$.

Proof. For each $G \in \tilde{\mathscr{G}}$ we may apply Proposition A.1.1 and thus $\psi_G \in K^G_{(\alpha - G(w))}$ is well defined in the statement of this lemma. We also have that

$$\begin{aligned} J(w + \psi_G) &= \frac{1}{2}a(w,w) + a(w,\psi_G) + \frac{1}{2}a(\psi_G,\psi_G) - l(w) - l(\psi_G) \\ &= J(w) + \frac{1}{2}a(\psi_G,\psi_G). \end{aligned}$$

Notice, by Proposition A.1.1 we have $a(\psi_G,\psi_G) = (A_G)^{-1}(\alpha - G(w)) \cdot (\alpha - G(w))$. By Proposition A.1.2 we may find a QPP global minimiser u and by our assumption $u \in K^F_\alpha$ for some $F \in \tilde{\mathscr{G}}$. As u minimises J over $L_\alpha \supset K^F_\alpha$ it follows

$$a(u,v) = l(v) \; \forall v \in K^F_0.$$

Hence $u - w \in K^F_{(\alpha - F(w))}$ and $a(u - w, v) = 0 \; \forall v \in K^F_0$, thus by uniqueness $u - w = \psi_F$. Now for any $G \in \tilde{\mathscr{G}}$, $w + \psi_G \in K^G_\alpha \subset L_\alpha$ hence

$$\begin{aligned} &J(u) = J(w) + \frac{1}{2}(A_F)^{-1}(\alpha - F(w)) \cdot (\alpha - F(w)), \\ &J(u) \leq J(w + \psi_G) = J(w) + \frac{1}{2}(A_G)^{-1}(\alpha - G(w)) \cdot (\alpha - G(w)). \end{aligned}$$

Thus $F \in \tilde{\mathscr{G}}$ is s.t

$$(A_F)^{-1}(\alpha - F(w)) \cdot (\alpha - F(w)) = \inf_{G \in \tilde{\mathscr{G}}} (A_G)^{-1}(\alpha - G(w)) \cdot (\alpha - G(w)).$$

Thus this infimum exists and is a minimum, completing the first part of the lemma. Now suppose u is any QPP global minimiser. By the above argument we have that $u = w + \psi_{F'}$ for some $F' \in \tilde{\mathscr{G}}$ which achieves the minimum of $G \mapsto (A_G)^{-1}(\alpha - G(w)) \cdot (\alpha - G(w))$.
For the backwards implication, suppose $F' \in \tilde{\mathscr{G}}$ and achieves the minimum value. Then $w + \psi_{F'} \in L_\alpha$ and by the above calculation, for any QPP global minimiser u

we have $J(w + \psi_{F'}) = J(u) \leq J(v)\ \forall v \in L_\alpha$. $\square$

To conclude this subsection we consider a minimization problem with parametrized source term $\mathcal{M} \ni y \to \ell_y(\,\cdot\,) \in V^*$.

Problem A.1.1 (Parametrized source term).
Find $(u, x) \in V \times \mathcal{M}$ minimizing the energy $J_x(u) = \frac{1}{2}a(u, u) - \ell_x(u)$ on $V \times \mathcal{M}$.

Existence is straightforward under appropriate assumptions on $x \mapsto l_x$ and $\mathcal{M}$.

Proposition A.1.3. *Assume that $\mathcal{M}$ is compact and that $\mathcal{M} \ni y \to \ell_y(\,\cdot\,) \in V^*$ is continuous. Then there is a solution $(u, x) \in V \times \mathcal{M}$ of Problem A.1.1.*

Proof. For each $x \in \mathcal{M}$ let u_x denote the unique solution to

$$a(u_x, v) = \ell_x(v)\ \forall v \in V.$$

For any $x, y \in \mathcal{M}$ observe, by the usual a priori bound for variational problems,

$$\|u_x - u_y\|_V \leq C\|\ell_x - \ell_y\|_{V^*},$$

hence the map $x \mapsto u_x$ is continuous and thus $x \mapsto J_x(u_x)$ is also continuous. Thus, by the compactness of $\mathcal{M}$ there exists $y \in \mathcal{M}$ minimising $J_x(u_x)$ over $\mathcal{M}$. Then for any $(u, x) \in V \times \mathcal{M}$

$$J_x(u) \geq J_x(u_x) \geq J_y(u_y),$$

hence (y, u_y) is the required minimiser. $\square$

A.2 Abstract penalisation method

We now introduce a penalisation method to recover the solution of the QPP as the limit of solutions to a family of similar minimisation problems over the whole space V.

Definition A.2.1 (Penalty method problem).
Using the notions in Definition A.1.1, let $\varepsilon > 0$ and u_ε be the unique minimiser over V of the functional given by

$$J_\varepsilon(v) := \frac{1}{2}a(v, v) - l(v) + \frac{1}{2\varepsilon}\sum_{j=1}^{N}\left(F_j(v) - \alpha_j\right)^2. \tag{A.1}$$

Such u_ε exist and are unique for each $\varepsilon > 0$ as J_ε is continuous, coercive and convex.
Note that J_ε is Gateaux differentiable, hence u_ε also satisfies

$$a(u_\varepsilon, v) - l(v) + \frac{1}{\varepsilon}\sum_{j=1}^{N} \left(F_j(u_\varepsilon) - \alpha_j\right) F_j(v) = 0 \;\; \forall v \in V.$$

Proposition A.2.1 (Recovery of quadratic programming problem in the limit)**.**
Let u be the unique minimiser solving the problem in Definition A.1.1 and u_ε be as in Definition A.2.1. Then $u_\varepsilon \to u$ in V as $\varepsilon \to 0$.

Proof. First notice, $u \in V$ and $F_j(u) = \alpha_j$ for each j, hence as u_ε is a minimiser of J_ε over V we have

$$\frac{C_c}{2}\|u_\varepsilon\|_V^2 - C_b\|u_\varepsilon\|_V \leq J_\varepsilon(u_\varepsilon) \leq J_\varepsilon(u) = \frac{1}{2}a(u,u) - l(u).$$

We thus have a uniform bound $\|u_\varepsilon\|_V \leq B$ for some $B > 0$. Now take any sequence $\varepsilon_n \to 0$ and subsequence $\varepsilon_{n'}$, by the above bound there exists a further subsequence $\varepsilon_{n''}$ and some $u_0 \in V$ such that $u_{\varepsilon_{n''}} \rightharpoonup u_0$ in V. For each $1 \leq j \leq N$ we have

$$\begin{aligned}
&\frac{1}{2}(F_j(u_{\varepsilon_{n''}}) - \alpha_j)^2 \leq \varepsilon_{n''} J_{\varepsilon_{n''}}(u_{\varepsilon_{n''}}) \leq \frac{\varepsilon_{n''}}{2}a(u,u) - \varepsilon_{n''} l(u),\\
\implies &\frac{1}{2}(F_j(u_0) - \alpha_j)^2 \leq 0.
\end{aligned}$$

Thus $F_j(u_0) = \alpha_j$ for each j and hence $u_0 \in K_\alpha^F$. Finally we see that, for any $w \in K_0^F$

$$\begin{aligned}
&a(u_{\varepsilon_{n''}}, w) - l(w) = -\frac{1}{\varepsilon_{n''}}\sum_{j=1}^{N}\left(F_j(u_{\varepsilon_{n''}}) - \alpha_j\right) F_j(w) = 0,\\
\implies &a(u_0, w) - l(w) = 0.
\end{aligned}$$

Thus $u_0 = u$ by the uniqueness of the minimiser u.
The norm values $\|u_{\varepsilon_{n''}}\|$ form a bounded sequence in $\mathbb{R}$ and so we may assume we chose the subsequence such that these norm values converge. By weak lower semi continuity of the norm in a Hilbert space we then have

$$\frac{1}{2}a(u,u) - l(u) \leq \lim_{n''\to\infty} \frac{1}{2}a(u_{\varepsilon_{n''}}, u_{\varepsilon_{n''}}) - l(u_{\varepsilon_{n''}}) \leq \frac{1}{2}a(u,u) - l(u).$$

We therefore have equality in the above thus $u_{\varepsilon_{n''}} \rightharpoonup u$ and $\|u_{\varepsilon_{n''}}\|_V \to \|u\|_V$ hence

$u_{\varepsilon_{n''}} \to u$ in V. Thus $u_{\varepsilon_n} \to u$ in V for any sequence $\varepsilon_n \to 0$. □

At this juncture we will also highlight the difference between soft constraints and hard constraints in these problems. Hard constraints are those that are forced to hold, as in QPP. Here we look for energy minimisers in the set where the constraints $F_j(v) = \alpha_j$ hold and so these constraints are forced upon the minimiser. Soft constraints are those that the system prefers but are not strictly enforced, as in the penalty method problem in Definition A.2.1. We look for minimisers of J_ε over the whole space V. Such a minimiser will be close to satisfying the constraints in the sense that the constraints hold in the limit, but the exact constraints need not hold for any $\varepsilon > 0$ necessarily.

Appendix B

Coercivity of Laplacian-based inner products

In this section we will prove the coercivity results for the Laplacian-based inner products, as required in sections 2.1.2 and 3.1.2. These results are also given in [38].

Lemma B.1.1. *Suppose $\Omega \subset \mathbb{R}^2$ is bounded with piecewise smooth boundary and take $V \subset H^2(\Omega)$ given by*

$$V = H_0^2(\Omega), \qquad V = H^2(\Omega) \cap H_0^1(\Omega), \qquad V = H_{p,0}^2(\Omega),$$

then $\|\Delta v\|_{0,2} = |v|_{2,2}$ for all $v \in V$. Note that for the final case we consider only rectangular domains Ω.

Proof. Let $\tilde{V} \subset V$ be a corresponding dense subspace of smooth functions given by

$$\tilde{V} = C_0^\infty(\overline{\Omega}), \qquad \tilde{V} = C^\infty(\mathbb{R}^2) \cap H_0^1(\Omega), \qquad \tilde{V} = C_{p,0}^\infty(\overline{\Omega}),$$

respectively. Note that it is sufficient to prove the result for dense subspaces. Introducing the piecewise smooth normal and tangential fields ν and τ, integration by parts yields

$$\begin{aligned}
\|\Delta v\|_{0,2}^2 &= |v|_{2,2}^2 + \sum_{i,j=1}^{2} \int_{\partial\Omega} \partial_i v \partial_{jj} v \nu_i - \partial_{ij} v \partial_i v \nu_j \, ds, \\
&= |v|_{2,2}^2 + \int_{\partial\Omega} \frac{\partial v}{\partial \nu} \Delta v - \nabla \frac{\partial}{\partial \nu} v \cdot \nabla v \, ds, \\
&= |v|_{2,2}^2 + \int_{\partial\Omega} \frac{\partial v}{\partial \nu} \frac{\partial^2}{\partial \tau^2} v - \frac{\partial^2}{\partial \tau \partial \nu} v \frac{\partial}{\partial \tau} v \, ds.
\end{aligned}$$

For each of the cases $\tilde{V} = C_0^\infty(\overline{\Omega}), \tilde{V} = C^\infty(\mathbb{R}^2) \cap H_0^1(\Omega)$ we have $v|_{\partial\Omega} = 0$ and thus the boundary integral is zero. For periodic boundary conditions the reversed orientation of the normal on opposite sides of the rectangle means their boundary integrals cancel out. □

Proposition B.1.2. *Suppose $\Omega \subset \mathbb{R}^2$ is bounded with piecewise smooth boundary and take $V \subset H^2(\Omega)$ given by*

$$V = H_0^2(\Omega), \qquad V = H^2(\Omega) \cap H_0^1(\Omega), \qquad V = H_{p,0}^2(\Omega),$$

then the the bilinear form $a(u, v) := \int_\Omega \Delta u \Delta v \, dx$ is coercive on V.

Proof. For each of the choices of V we have a Poincaré inequality

$$\exists C_V > 0 \text{ such that } \|v\|_{0,2} \leq C_V |v|_{H^1(\Omega)} \quad \forall v \in V.$$

We can also use integration by parts to obtain

$$|v|_{1,2}^2 = \int_\Omega -v\Delta v \, dx \leq \|v\|_{0,2}\|\Delta v\|_{0,2} \leq C_V |v|_{1,2}\|\Delta v\|_{0,2}, \tag{B.1}$$

hence we have the Poincaré-type inequality

$$|v|_{1,2} \leq C_V \|\Delta v\|_{0,2}.$$

Hence we have coercivity as

$$\|v\|_{2,2}^2 = \|v\|_{0,2}^2 + |v|_{1,2} + |v|_{2,2} \leq (C_V^4 + C_V^2 + 1)a(v, v).$$

□

This is the required coercivity result for Section 2.1.2, we now derive analogous results for the eighth order problem, in a $H^4(\Omega)$ setting.

Lemma B.1.2. *Suppose $\Omega \subset \mathbb{R}^2$ is bounded with piecewise smooth boundary and take $V \subset H^4(\Omega)$ given by*

$$V = H^4(\Omega) \cap H_0^3(\Omega), \quad V = \left\{ v \in H^4(\Omega) \mid v = \Delta v = 0 \text{ on } \partial\Omega \right\}, \quad V = H_{p,0}^4(\Omega),$$

then $\|\Delta^2 v\|_{0,2} = |v|_{4,2}$ for all $v \in V$. Note that for the final two cases we consider only rectangular domains Ω.

Proof. Let $\tilde{V} \subset V$ be a corresponding dense subspace of smooth functions given by $C^\infty(\mathbb{R}^2) \cap H_0^3(\Omega)$, $\left\{v \in C^\infty(\mathbb{R}^2) \mid v = \Delta v = 0 \text{ on } \partial\Omega\right\}$ or $C^\infty_{p,0}(\overline{\Omega})$ respectively. Now for $v \in \tilde{V}$ consider $w = \Delta v \in H^2(\Omega)$, for each case we can apply Lemma B.1.1 to get

$$\|\Delta^2 v\|_{0,2} = |\Delta v|_{2,2}^2 = \sum_{|s|=2} \|D^s \Delta v\|_{0,2}^2 = \sum_{|s|=2} \|\Delta D^s v\|_{0,2}^2.$$

Hence it remains to show $\|\Delta z\|_{0,2}^2 = |z|_{2,2}^2$ for $z = D^s v$ and $|s| = 2$. To this end we integrate by parts as in Lemma B.1.1 to get

$$\|\Delta z\|_{0,2}^2 = |z|_{2,2}^2 + \int_{\partial\Omega} \frac{\partial z}{\partial \nu} \frac{\partial^2}{\partial \tau^2} z - \frac{\partial^2}{\partial \tau \partial \nu} z \frac{\partial}{\partial \tau} z \, ds. \tag{B.2}$$

For $v \in C^\infty(\mathbb{R}^2) \cap H_0^3(\Omega)$, $z|_{\partial\Omega} = 0$ hence the boundary integral vanishes. For periodic boundary conditions on a rectangular domain the boundary integral vanishes by the same arguments as in Lemma B.1.1. We are thus left with $v \in \left\{v \in C^\infty(\mathbb{R}^2) \mid v = \Delta v = 0 \text{ on } \partial\Omega\right\}$ with Ω a rectangular domain. In this case the boundary $\partial\Omega$ is a set of straight lines, each one parallel to one of the coordinate axes. It follows, on each section of the boundary, the only possibilities for z are

$$z = \frac{\partial^2 v}{\partial \tau \partial \tau}, \; z = \frac{\partial^2 v}{\partial \nu \partial \nu} \text{ or } z = \frac{\partial^2 v}{\partial \tau \partial \nu}.$$

For the first two cases $z|_{\partial\Omega} = 0$ by the conditions $v = \Delta v = 0$ on $\partial\Omega$. For the remaining case observe

$$\frac{\partial z}{\partial \nu} = \frac{\partial}{\partial \tau}\left(\frac{\partial^2 v}{\partial \nu \partial \nu}\right) \text{ and } \frac{\partial^2 z}{\partial \tau \partial \nu} = \frac{\partial^2}{\partial \tau \partial \tau}\left(\frac{\partial^2 v}{\partial \nu \partial \nu}\right).$$

Each of these terms vanishes along the boundary due to the boundary conditions $v = \Delta v = 0$, hence the boundary integral vanishes. □

Proposition B.1.3. *Suppose $\Omega \subset \mathbb{R}^2$ is bounded with piecewise smooth boundary and take $V \subset H^2(\Omega)$ given by*

$$V = H^4(\Omega) \cap H_0^3(\Omega), \quad V = \left\{v \in H^4(\Omega) \mid v = \Delta v = 0 \text{ on } \partial\Omega\right\}, \quad V = H^2_{p,0}(\Omega),$$

then the bilinear form $a(u,v) := \int_\Omega \Delta^2 u \Delta^2 v \, dx$ is coercive on V. Note that for the final two cases we consider only rectangular domains Ω.

Proof. Observe

$$\int_\Omega |\nabla \Delta v|^2 \, dxdy - |v|_{3,2}^2 = 2\int_\Omega v_{xxx} v_{xyy} + v_{xxy} v_{yyy} - (v_{xxy}^2 + v_{xyy}^2) \, dxdy.$$

Working with the dense subspaces of smooth functions from the previous lemma and integrating by parts it follows

$$\begin{aligned}\int_\Omega v_{xxx}v_{xyy}\,dxdy &= \int_\Omega -v_{xx}v_{xxyy}\,dxdy + \int_{\partial\Omega} v_{xx}v_{xyy}\nu_1\,ds\\ &= \int_\Omega v_{xxy}^2 + \int_{\partial\Omega} v_{xx}\partial_\tau(v_{xy})\,ds.\end{aligned}$$

Similarly, interchanging x and y produces

$$\int_\Omega v_{xyy}v_{yyy}\,dxdy = \int_\Omega v_{xyy}^2 + \int_{\partial\Omega} v_{yy}\partial_\tau(v_{xy})\,ds.$$

It follows

$$\int_\Omega |\nabla\Delta v|^2\,dxdy - |v|_{3,2}^2 = \int_{\partial\Omega} \Delta v\partial_\tau(v_{xy})\,ds.$$

For the non-periodic boundary conditions $\Delta v|_{\partial\Omega} = 0$ hence this boundary integral vanishes. For the periodic boundary conditions on a rectangular domain note that the direction of τ is opposite on opposite boundaries, hence the boundary integral vanishes in this case also. A similar argument to (B.1) together with Lemma B.1.2 produces the Poincaré-type inequalities

$$\|v\|_{L^2(\Omega)} \le C_V|v|_{H^1(\Omega)}C_V^2|v|_{H^2(\Omega)} \le C_V^3|v|_{H^3(\Omega)} \le C_V^4|v|_{H^3(\Omega)} = C_V^4 a(v,v).$$

Coercivity is immediate from these inequalities. $\square$

Appendix C

Regularity for problems with delta right hand side

Here we will collect regularity results for fourth and eighth order problems where the right hand side is a delta function. These results can be applied to study regularity of the solutions to several problems posed in Chapter 2 and Chapter 3. These include Problem 2.3.1, related to point forces, and the two point constraints problems (Problem 2.2.1 and Problem 3.2.1). The results presented are for particular choices of domains and boundary conditions. Specifically, we consider the domains and boundary conditions for which we employ a numerical method based on splitting. These regularity results ensure the well posedness of such splitting methods. We begin with the fourth order problem.

C.1 Fourth order problems

Lemma C.1.1. *Suppose $\Omega \subset \mathbb{R}^2$ is a convex, bounded domain with Lipschitz boundary. Let $X \in \Omega$ and $V = H^2(\Omega) \cap H_0^1(\Omega)$. Let $a_1 > 0, a_2, a_3 \geq 0$ and define a bilinear form $a(\cdot,\cdot) : V \times V \to \mathbb{R}$ by*

$$a(u,v) = \int_\Omega a_1 \Delta u \Delta v + a_2 \nabla u \cdot \nabla v + a_3 uv \, dx.$$

Let $u \in V$ be the unique solution such that

$$a(u,v) = v(X) \; \forall v \in V.$$

Then $-\Delta u \in W^{1,s}(\Omega)$ for any $s \in (1,2)$. If $\partial\Omega$ is smooth we also have the additional regularity $u \in W^{3,s}(\Omega)$ for any $s \in (1,2)$.

Proof. We first prove the result for $a_3 = 0$, in this case set $-\Delta u =: w \in L^2(\Omega)$ and for any $v \in V$ it holds

$$v(X) = \int_\Omega a_1 \Delta u \Delta v + a_2 \nabla u \cdot \nabla v \; dx = \int_\Omega w(-a_1 \Delta v + a_2 v) \; dx.$$

Hence by [14] we have $w \in W^{1,s}(\Omega)$ for any $s \in (1,2)$. When the boundary is smooth the final result follows by elliptic regularity, $u \in W^{3,s}(\Omega)$ for any $s \in (1,2)$, see for example [45]. Now we extend to $a_3 \geq 0$. Let $p, q \in V$ denote the unique solutions to

$$\int_\Omega a_1 \Delta p \Delta v + a_2 \nabla p \cdot \nabla v \; dx = v(x) \; \forall v \in V,$$
$$\int_\Omega a_1 \Delta q \Delta v + a_2 \nabla q \cdot \nabla v + a_3 q v \; dx = \int_\Omega -a_3 p v \; dx \; \forall v \in V.$$

It is then clear $u = p + q$. For any $s \in (1,2)$ we have $-\Delta p \in W^{1,s}(\Omega)$ by the above. Furthermore $-\Delta q \in L^2(\Omega)$ and satisfies

$$\int_\Omega -\Delta q(-a_1 \Delta v + a_2 v) \; dx = \int_\Omega -a_3(p+q) v \; dx \; \forall v \in V.$$

By [14], $(-a_1\Delta + a_2)$ is an isomorphism from V onto $L^2(\Omega)$ and by the above equation it follows $-\Delta q = (-a_1 \Delta + a_2)^{-1}[-a_3(p+q)] \in V$. Hence $-\Delta u = -\Delta p + -\Delta q \in W^{1,s}(\Omega)$ for any $s \in (1,2)$. When the boundary is smooth the final result again follows by elliptic regularity, $u \in W^{3,s}(\Omega)$ for any $s \in (1,2)$. □

We now produce a similar result for the eighth order problem.

C.2 Eighth order problems

Lemma C.2.1. *Suppose $\Omega \subset \mathbb{R}^2$ is a bounded rectangle, $\Omega = (0,L) \times (0,M)$ for some $L, M > 0$. Let $X \in \Omega$ and $V = \left\{ v \in H^4(\Omega) \mid v = \Delta v = 0 \text{ on } \partial\Omega \right\}$. Let $a_1 > 0, a_2, a_3, a_4, a_5 \geq 0$ and define a bilinear form $a(\cdot, \cdot) : V \times V \to \mathbb{R}$ by*

$$a(u,v) = \int_\Omega a_1 \Delta^2 u \Delta^2 v + a_2 \nabla \Delta u \cdot \nabla \Delta v + a_3 \Delta u \Delta v + a_4 \nabla u \cdot \nabla v + a_5 u v \; dx.$$

Let $u \in V$ be the unique solution such that

$$a(u,v) = \Delta v(X) \; \forall v \in V. \tag{C.1}$$

Then $\Delta^2 u \in W_0^{1,s}(\Omega)$ for any $s \in (1,2)$.

Proof. We begin with the case $a_3 = a_4 = a_5 = 0$. Define the set $\Delta V := \{\Delta v \mid v \in V\}$, observe ΔV contains each of the eigenfunctions of the Dirichlet Laplacian. We now show ΔV is dense in $H^2(\Omega) \cap H_0^1(\Omega)$, first note

$$\overline{\Delta V} = (\Delta V)^{\perp\perp},$$

where orthogonality is taken with respect to the $H^2(\Omega) \cap H_0^1(\Omega)$ inner product

$$\langle u, v\rangle = \int_\Omega \Delta u \Delta v \; dx.$$

Hence if $g \in (\Delta V)^\perp$ then for any eigenfunction e_i, with eigenvalue λ_i,

$$0 = \int_\Omega \Delta g \Delta e_i \; dx = \lambda_i^2 \int_\Omega g e_i \; dx.$$

That is g is orthogonal to each eigenfunction with respect to the $L^2(\Omega)$ inner product also. Since the eigenfunctions are dense in $L^2(\Omega)$ we have $g = 0$, thus $(\Delta V)^\perp = \{0\}$ and hence

$$\overline{\Delta V} = \{0\}^\perp = H^2(\Omega) \cap H_0^1(\Omega). \tag{C.2}$$

Integrating (C.1) by parts produces

$$\int_\Omega \Delta^2 u(a_1\Delta^2 v - a_2\Delta v) \; dx = \Delta v(X) \; \forall v \in V$$

which implies

$$\int_\Omega \Delta^2 u(-a_1\Delta v + a_2 v) \; dx = -v(X) \; \forall v \in \Delta V.$$

The above equation may be extended to any $v \in H^2(\Omega) \cap H_0^1(\Omega)$ by using the density result outlined previously. Then $\Delta^2 u \in W_0^{1,s}(\Omega)$, using the same result of [14] as in the previous lemma.

To extend to $(a_3, a_4, a_5) \neq (0, 0, 0)$ consider $p, q \in V$ solving

$$\int_\Omega a_1\Delta^2 u\Delta^2 v + a_2\nabla\Delta u \cdot \nabla\Delta v \; dx = \Delta v(X) \; \forall v \in V,$$
$$a(q, v) = \int_\Omega (-a_3\Delta^2 p + a_4\Delta p - a_5 p)v \; dx \; \forall v \in V.$$

Integrating the right hand side of the second equation by parts shows $u = p + q$. By the above $\Delta^2 p \in W_0^{1,s}(\Omega)$ for any $s \in (0,1)$. Observe

$$\int_\Omega \Delta^2 q(a_1\Delta^2 v - a_2\Delta v)\ dx = \int_\Omega (-a_3\Delta^2(p+q) + a_4\Delta(p+q) - a_5(p+q))v\ dx\ \forall v \in V.$$

Let $\psi \in H^2(\Omega) \cap H_0^1(\Omega)$ denote the solution to

$$\int_\Omega a_1\Delta\psi\Delta v + a_2\nabla\psi\cdot\nabla v\ dx = \int_\Omega (-a_3\Delta^2(p+q) + a_4\Delta(p+q) - a_5(p+q))v\ dx\ \forall v \in H^2(\Omega)\cap H_0^1(\Omega).$$

Integrating by parts, it follows

$$\int_\Omega (\psi - \Delta^2 q)(-a_1\Delta v + a_2 v)\ dx = 0\ \forall v \in \Delta V.$$

This equation can be extended to all $v \in H^2(\Omega) \cap H_0^1(\Omega)$ by the density result (C.2). Then $\psi - \Delta^2 q = 0$ as $(-a_1\Delta + a_2)$ is an isomorphism from $H^2(\Omega)$ onto $L^2(\Omega)$. Thus $\Delta^2 q \in H^2(\Omega) \cap H_0^1(\Omega)$ and hence $\Delta^2 u \in W_0^{1,s}(\Omega)$ for any $s \in (0,1)$. $\square$

We require the following lemma for the calculations in Section 3.2.3.

Lemma C.2.2. *Let $X \in \mathbb{R}^2$, fix $a_1, a_2, a_3, a_4, a_5 > 0$ and define a bilinear form $a(\cdot,\cdot) : H^4(\mathbb{R}^2) \times H^4(\mathbb{R}^2) \to \mathbb{R}$ by*

$$a(u,v) = \int_{\mathbb{R}^2} a_1\Delta^2 u\Delta^2 v + a_2\nabla\Delta u\cdot\nabla\Delta v + a_3\Delta u\Delta v + a_4\nabla u\cdot\nabla v + a_5 uv\ dx$$

Let $u \in H^4(\mathbb{R}^2)$ be the unique solution s.t.

$$a(u,v) = v(X)\ \forall v \in H^4(\mathbb{R}^2).$$

Then $u \in H^s(\mathbb{R}^2)$ for any $s \in (0,7)$.

Proof. Without loss of generality take $X = 0$ as solutions for $X \neq 0$ will be translations of this case. Let $\mathcal{F} : L^2(\mathbb{R}^2) \to L^2(\mathbb{R}^2)$ denote the Fourier transform which is the continuous extension of

$$\mathcal{F}[\varphi](\xi) := \int_{\mathbb{R}^2} \varphi(x)e^{-2\pi i\xi\cdot x}\ dx,\ \text{for } \varphi \in C_0^\infty(\mathbb{R}^2).$$

Define

$$f(\xi) := \left[a_1(4\pi^2|\xi|^2)^4 + a_2(4\pi^2|\xi|^2)^3 + a_3(4\pi^2|\xi|^2)^2 + a_4(4\pi^2|\xi|^2) + a_5\right]^{-1}.$$

Notice $f \in L^2(\mathbb{R}^2)$, thus define $g := \mathcal{F}^{-1}[f] \in L^2(\mathbb{R}^2)$. For $s < 7$ it follows

$$\int_{\mathbb{R}^2} (1 + |\xi|^2)^s |\mathcal{F}[g](\xi)|^2 \, d\xi = 2\pi \int_0^\infty (1 + r^2)^s |f((r, 0))|^2 r \, dr < \infty$$

as the final integrand is continuous and behaves as r^{2s-15} for large r. This is integrable provided $2s - 15 < -1$, that is $s < 7$. Hence $g \in H^s(\mathbb{R}^2)$ for $s < 7$, in particular $g \in H^4(\mathbb{R}^2)$.

Now let $\varphi \in C_0^\infty(\mathbb{R}^2)$, then by Parseval's formula

$$\begin{aligned} a(g, \varphi) &= \int_{\mathbb{R}^2} \left[a_1(4\pi^2|\xi|^2)^4 + a_2(4\pi^2|\xi|^2)^3 + a_3(4\pi^2|\xi|^2)^2 + a_4(4\pi^2|\xi|^2) + a_5\right] \mathcal{F}[g]\mathcal{F}[\varphi] \, d\xi \\ &= \int_{\mathbb{R}^2} \mathcal{F}[\varphi] \, d\xi \\ &= \delta_0(\varphi) \end{aligned}$$

As $C_0^\infty(\mathbb{R}^2)$ is dense in $H^4(\mathbb{R}^2)$ and $\delta_0 : H^4(\mathbb{R}^2) \to \mathbb{R}$ is continuous it follows $a(g, v) = v(0) \; \forall v \in H^4(\mathbb{R}^2)$. Thus $u = g \in H^s(\mathbb{R}^2)$ for $s < 7$. $\square$

Appendix D

Second variation formulas on surfaces

Derivation of the second variation of the Willmore functional

For the sake of completeness we present the derivation of the second variation of The Willmore functional and other functionals required in Chapter 4, see also [35]. We will not integrate by parts in the formulas below – unless otherwise stated. This means that our results can be more readily adapted to surfaces with boundary. This might be useful for studying biomembranes with finite-size inclusions. The following calculations are valid for n-dimensional hypersurfaces $\Gamma \subset \mathbb{R}^{n+1}$. We begin by calculating the required material derivatives, starting with the unit normal.

Lemma D.1.1. *Suppose $\Gamma \subset \mathbb{R}^{n+1}$ is a parametrised n-dimensional hypersurface, $\Gamma = \{X(\theta) \mid \theta \in \Omega\}$, let $u \in C^1(\Gamma)$ and define*

$$\Gamma_\mu := \{X^\mu(\theta) := X(\theta) + \mu\tilde{u}(\theta)\tilde{\nu}(\theta) \mid \theta \in \Omega\}$$

where $\tilde{u}(\theta) := u(X(\theta))$ and $\tilde{\nu}(\theta) := \nu(X(\theta))$. Then the material derivative of the normal is given by

$$\dot{\partial}\nu^\mu = -\nabla_\Gamma u.$$

Proof. We have

$$0 = \dot{\partial}\left(|\nu^\mu|^2\right) = 2\nu \cdot \dot{\partial}(\nu^\mu)$$

thus $\dot{\partial}(\nu^\mu) \in \nu^\perp$ so let $\dot{\partial}(\nu^\mu) \circ X = \sum_{i=1}^n \alpha_i X_{\theta_i}$. It then follows

$$\sum_{i=1}^n \alpha_i g_{ij} = \left(\dot{\partial}(\nu^\mu) \circ X\right) \cdot X_{\theta_j} = -\left(\dot{\partial}(X^\mu_{\theta_j})\right) \cdot \tilde{\nu} = -\tilde{\nu} \cdot (\tilde{u}\tilde{\nu})_{\theta_j} = -\tilde{u}_{\theta_j}.$$

We may then conclude

$$\dot{\partial}(\nu^\mu) \circ X = \sum_{i=1}^{n} \alpha_i X_{\theta_i} = \sum_{i,j,k=1}^{n} \alpha_i g_{ik} g^{jk} X_{\theta_j} = -\sum_{j,k=1}^{n} g^{jk} \tilde{u}_{\theta_k} X_{\theta_j} = -\nabla_\Gamma u \circ X.$$

□

Now we will calculate the material derivative for the entries of the inverse of the first fundamental form.

Lemma D.1.2. *Denote the entries of the inverse of the first fundamental form G^μ by $g^{\mu ij}$, then*

$$\dot{\partial} g^{\mu ij} = -\sum_{k,l=1}^{n} \tilde{u} g^{il} g^{kj} (X_{\theta_k} \cdot \tilde{\nu}_{\theta_l} + X_{\theta_l} \cdot \tilde{\nu}_{\theta_k}).$$

Proof.

$$\begin{aligned}
\dot{\partial} g^{\mu ij} &= \dot{\partial} \left(\sum_{k,l=1}^{n} g^{\mu kj} g^{\mu li} g^\mu_{lk} \right) \\
&= \sum_{k=1}^{n} \left(\dot{\partial} g^{\mu kj} \right) \delta^i_k + \sum_{l=1}^{n} \left(\dot{\partial} g^{\mu li} \right) \delta^j_l + \sum_{k,l=1}^{n} g^{kj} g^{li} \left(\dot{\partial} g^\mu_{lk} \right) \\
&= 2\dot{\partial} g^{\mu ij} + \sum_{k,l=1}^{n} \tilde{u} g^{kj} g^{li} (X_{\theta_k} \cdot \tilde{\nu}_{\theta_l} + X_{\theta_l} \cdot \tilde{\nu}_{\theta_k}).
\end{aligned}$$

□

Next, we will derive the material derivative of the tangential gradient.

Lemma D.1.3. *Suppose Γ, Γ_μ are as in Lemma D.1.1 and let $f^\mu : \Gamma_\mu \to \mathbb{R}$ then*

$$\dot{\partial} \left(\nabla_{\Gamma^\mu} f^\mu \right) = -u \mathcal{H} \nabla_\Gamma f + (\nabla_\Gamma f \cdot \nabla_\Gamma u) \nu + \nabla_\Gamma \left(\dot{\partial} f^\mu \right).$$

Proof.

$$\begin{aligned}
&\dot{\partial}\left(\nabla_{\Gamma^\mu} f^\mu\right)\circ X = \dot{\partial}\left(\sum_{i,j=1}^{n} g^{\mu ij}\tilde{f}^\mu_{\theta_i}X^\mu_{\theta_j}\right)\\
&= -\sum_{i,j,k,l=1}^{n} \tilde{u}g^{kj}g^{li}(X_{\theta_k}\cdot\tilde{\nu}_{\theta_l}+X_{\theta_l}\cdot\tilde{\nu}_{\theta_k})\tilde{f}_{\theta_i}X_{\theta_j} + \sum_{i,j=1}^{n}\left(g^{ij}\tilde{f}_{\theta_i}\dot{\partial}X^\mu_{\theta_j}+g^{ij}X_{\theta_j}\dot{\partial}\left(\tilde{f}^\mu\right)_{\theta_i}\right)\\
&= -\sum_{i,l=1}^{n}\sum_{\gamma=1}^{n+1}\tilde{u}g^{il}\tilde{f}_{\theta_i}\tilde{\nu}_{\gamma\theta_l}\nabla_\Gamma X_\gamma - \tilde{u}(\mathcal{H}\nabla_\Gamma f)\circ X + \sum_{i,j=1}^{n} g^{ij}\tilde{f}_{\theta_i}\left(\tilde{u}_{\theta_j}\tilde{\nu}+\tilde{u}\tilde{\nu}_{\theta_j}\right)\\
&\quad + \nabla_\Gamma\left(\dot{\partial}f^\mu\right)\circ X\\
&= \left(-u\mathcal{H}\nabla_\Gamma f + (\nabla_\Gamma f\cdot\nabla_\Gamma u)\nu + \nabla_\Gamma\left(\dot{\partial}f^\mu\right)\right)\circ X.
\end{aligned}$$

□

These three lemmas combined produce the following calculations.

Corollary D.1.1. *The mean curvature $H^\mu = \nabla_{\Gamma^\mu}\cdot\nu^\mu$ satisfies*

$$\dot{\partial}H^\mu = -\Delta_\Gamma u - |\mathcal{H}|^2 u.$$

The extended Weingarten map $\mathcal{H}^\mu = \nabla_{\Gamma^\mu}\nu^\mu$ satisfies

$$\dot{\partial}\left(|\mathcal{H}^\mu|^2\right) = -2uTr\left(\mathcal{H}^3\right) - 2\mathcal{H}:\nabla_\Gamma\nabla_\Gamma u.$$

Proof. By Lemma D.1.3 it holds, for each $1\le\alpha\le n+1$,

$$\dot{\partial}\left(\nabla_{\Gamma^\mu}\nu^\mu_\alpha\right) = -u\mathcal{H}\nabla_\Gamma\nu_\alpha + (\nabla_\Gamma\nu_\alpha\cdot\nabla_\Gamma u)\nu + \nabla_\Gamma\left(\dot{\partial}\nu^\mu_\alpha\right).$$

Applying Lemma D.1.1 to the final term then gives

$$\dot{\partial}\left(\nabla_{\Gamma^\mu}\nu^\mu_\alpha\right) = -u\mathcal{H}\nabla_\Gamma\nu_\alpha + (\nabla_\Gamma\nu_\alpha\cdot\nabla_\Gamma u)\nu - \nabla_\Gamma\underline{D}_\alpha u.$$

Hence, for the mean curvature,

$$\begin{aligned}
\dot{\partial}(H^\mu) &= \sum_{\alpha=1}^{n+1}\dot{\partial}\left(D^{\Gamma^\mu}_\alpha\nu^\mu_\alpha\right)\\
&= \sum_{\alpha,\beta=1}^{n+1} -u\mathcal{H}_{\alpha\beta}\mathcal{H}_{\alpha\beta} + \mathcal{H}_{\alpha\beta}\underline{D}_\beta u\nu_\alpha - \underline{D}_\alpha\underline{D}_\alpha u\\
&= -|\mathcal{H}|^2u - \Delta_\Gamma u.
\end{aligned}$$

Similarly, for the squared Frobenius norm of $\mathcal{H}$,

$$\begin{aligned}
\dot{\partial}\left(|\mathcal{H}^\mu|^2\right) &= \sum_{\alpha,\beta=1}^{n+1} 2\mathcal{H}_{\alpha\beta}\dot{\partial}(\underline{D}_\beta\nu_\alpha) \\
&= \sum_{\alpha,\beta,\gamma=1}^{n+1} 2\mathcal{H}_{\alpha\beta}\left(-u\mathcal{H}_{\beta\gamma}\mathcal{H}_{\gamma\alpha} + \mathcal{H}_{\gamma\alpha}\underline{D}_\gamma u\nu_\beta - \underline{D}_\beta\underline{D}_\alpha u\right) \\
&= 2Tr(\mathcal{H}^3) - 2\mathcal{H} : \nabla_\Gamma\nabla_\Gamma u.
\end{aligned}$$

□

We may now calculate the final material derivative required for the second variation.

Lemma D.1.4. *For the material derivative of $\Delta_{\Gamma^\mu} f^\mu$ we have*

$$\begin{aligned}
\dot{\partial}\left(\Delta_{\Gamma^\mu} f^\mu\right) = -2u\mathcal{H} : \nabla_\Gamma\nabla_\Gamma f - 2\mathcal{H}\nabla_\Gamma f\cdot\nabla_\Gamma u - u\nabla_\Gamma f\cdot\nabla_\Gamma H \\
+ H\nabla_\Gamma f\cdot\nabla_\Gamma u + \Delta_\Gamma\left(\dot{\partial} f^\mu\right).
\end{aligned}$$

Proof. Using the commutator rule in (4.1), we obtain

$$\begin{aligned}
&\dot{\partial}\left(\Delta_{\Gamma^\mu} f^\mu\right) = \sum_{\alpha=1}^{n+1} -u\nabla_\Gamma\underline{D}_\alpha f\cdot\nabla_\Gamma\nu_\alpha + \sum_{\alpha,\beta=1}^{n+1}\nu_\alpha\underline{D}_\beta\underline{D}_\alpha f\underline{D}_\beta u + \sum_{\alpha=1}^{n+1}\underline{D}_\alpha\left(\dot{\partial}\underline{D}^\mu_\alpha f^\mu\right) \\
&= -u\mathcal{H} : \nabla_\Gamma\nabla_\Gamma f + \sum_{\alpha,\beta=1}^{n+1}\left(\nu_\alpha\underline{D}_\alpha\underline{D}_\beta f\underline{D}_\beta u + \sum_{\gamma=1}^{n+1}\nu_\alpha\underline{D}_\beta u\left(\nu_\beta\underline{D}_\alpha\nu_\gamma\underline{D}_\gamma f - \nu_\alpha\underline{D}_\beta\nu_\gamma\underline{D}_\gamma f\right)\right) \\
&\quad + \sum_{\alpha,\beta=1}^{n+1} -\underline{D}_\alpha\left(u\underline{D}_\beta f\underline{D}_\beta\nu_\alpha\right) + \underline{D}_\alpha(\nu_\alpha\underline{D}_\beta f\underline{D}_\beta u) + \underline{D}_\alpha\underline{D}_\alpha\left(\dot{\partial} f^\mu\right) \\
&= -2u\mathcal{H} : \nabla_\Gamma\nabla_\Gamma f - 2\mathcal{H}\nabla_\Gamma f\cdot\nabla_\Gamma u - u\nabla_\Gamma f\cdot\nabla_\Gamma H + H\nabla_\Gamma f\cdot\nabla_\Gamma u + \Delta_\Gamma\left(\dot{\partial} f^\mu\right)
\end{aligned}$$

where in the last step we have made use of the identity

$$\sum_{\alpha=1}^{n+1}\underline{D}_\alpha\underline{D}_\beta\nu_\alpha = \underline{D}_\beta H - |\mathcal{H}|^2\nu_\beta.$$

□

We now use these results to calculate the second variation of the Willmore functional:

$$W(\Gamma) := \frac{1}{2}\int_\Gamma H^2\, do$$

which has first variation, via the transport formula (4.3), given by

$$W'(\Gamma)[u\nu] = \int_\Gamma H\dot{\partial}\left(H^\mu\right) + \frac{1}{2}H^3 u \, do = \int_\Gamma -H\Delta_\Gamma u - H|\mathcal{H}|^2 u + \frac{1}{2}H^3 u \, do. \quad \text{(D.1)}$$

Theorem D.1.1. *The second variation of the Willmore functional $W(\Gamma)$ is given by*

$$\begin{aligned} W''(\Gamma)[u\nu, g\nu] = &\int_\Gamma (\Delta_\Gamma g + |\mathcal{H}|^2 g)(\Delta_\Gamma u + |\mathcal{H}|^2 u) + 2H\mathcal{H} : (g\nabla_\Gamma\nabla_\Gamma u + u\nabla_\Gamma\nabla_\Gamma g) \\ &+ 2H\mathcal{H}\nabla_\Gamma u \cdot \nabla_\Gamma g + Hg\nabla_\Gamma u \cdot \nabla_\Gamma H - H^2\nabla_\Gamma u \cdot \nabla_\Gamma g - \frac{3}{2}H^2 u\Delta_\Gamma g - H^2 g\Delta_\Gamma u \\ &+ \left(2HTr(\mathcal{H}^3) - \frac{5}{2}H^2|\mathcal{H}|^2 + \frac{1}{2}H^4\right) gu \, do. \end{aligned}$$

Proof. We use the transport formula again and note that u is extended constantly in the normal direction, in accordance with Remark 4.2.2.

$$\begin{aligned} W''(\Gamma)[u\nu, g\nu] = \int_\Gamma &-(\dot{\partial}H^\mu)(\Delta_\Gamma u + |\mathcal{H}|^2 u) - H\dot{\partial}(\Delta_{\Gamma^\mu} u^\mu) - H\dot{\partial}(|\mathcal{H}^\mu|^2)u \\ &+ \frac{3}{2}H^2(\dot{\partial}H^\mu)u - H^2 g\Delta_\Gamma u - H^2|\mathcal{H}|^2 gu + \frac{1}{2}H^4 gu \, do \end{aligned}$$

Using the results of the above lemmas to calculate the required material derivatives produces the result. □

Remark D.1.1. *Using integration by parts on closed surfaces for the term*

$$\begin{aligned} \int_\Gamma Hg\nabla_\Gamma u \cdot \nabla_\Gamma H \, do &= \int_\Gamma \nabla_\Gamma u \cdot \nabla_\Gamma\left(\frac{1}{2}H^2 g\right) - \frac{1}{2}H^2\nabla_\Gamma u \cdot \nabla_\Gamma g \, do \\ &= \int_\Gamma -\frac{1}{2}H^2 g\Delta_\Gamma u - \frac{1}{2}H^2\nabla_\Gamma u \cdot \nabla_\Gamma g \, do \end{aligned}$$

leads to

$$\begin{aligned} W''(\Gamma)[u\nu, g\nu] = &\int_\Gamma (\Delta_\Gamma g + |\mathcal{H}|^2 g)(\Delta_\Gamma u + |\mathcal{H}|^2 u) + 2H\mathcal{H} : (g\nabla_\Gamma\nabla_\Gamma u + u\nabla_\Gamma\nabla_\Gamma g) \\ &+ 2H\mathcal{H}\nabla_\Gamma u \cdot \nabla_\Gamma g - \frac{3}{2}H^2\nabla_\Gamma u \cdot \nabla_\Gamma g - \frac{3}{2}H^2(u\Delta_\Gamma g + g\Delta_\Gamma u) \qquad \text{(D.2)} \\ &+ \left(2HTr(\mathcal{H}^3) - \frac{5}{2}H^2|\mathcal{H}|^2 + \frac{1}{2}H^4\right) gu \, do \end{aligned}$$

which unveils the symmetry of the second variation.

Corollary D.1.2. *If $\Gamma = S(0, R)$, an $n-$sphere, then the second variation of the*

Willmore functional $W(\Gamma)$ is given by

$$W''(\Gamma)[u\nu, g\nu] = \int_\Gamma \Delta_\Gamma g \Delta_\Gamma u + \frac{n}{R^2}\left(\frac{3n}{2} - 4\right)\nabla_\Gamma g \cdot \nabla_\Gamma u + \frac{n^2}{R^4}\left(\frac{n^2}{2} - \frac{5n}{2} + 3\right) gu \, do.$$

Proof. Inserting $\mathcal{H} = \frac{1}{R}P$ and $H = \frac{n}{R}$ into the second variation and using integration by parts produces the result. □

For the numerical method used in Section 4.6.6 we use the bilinear form

$$\begin{aligned} t(u,g) :&= W''(\Gamma)[u\nu, g\nu] - \int_\Gamma (-\Delta_\Gamma g + g)(-\Delta_\Gamma u + u) \, do \\ &= \int_\Gamma (\Delta_\Gamma g + |\mathcal{H}|^2 g)(\Delta_\Gamma u + |\mathcal{H}|^2 u) - (-\Delta_\Gamma g + g)(-\Delta_\Gamma u + u) \\ &\quad + 2H\mathcal{H} : (g\nabla_\Gamma\nabla_\Gamma u + u\nabla_\Gamma\nabla_\Gamma g) + 2H\mathcal{H}\nabla_\Gamma g \cdot \nabla_\Gamma u \\ &\quad - \frac{3}{2}H^2 \nabla_\Gamma g \cdot \nabla_\Gamma u - \frac{3}{2}H^2(g\Delta_\Gamma u + u\Delta_\Gamma g) \\ &\quad + \left(2HTr(\mathcal{H}^3) - \frac{5}{2}H^2|\mathcal{H}|^2 + \frac{1}{2}H^4\right) uv \, do. \end{aligned} \tag{D.3}$$

The reasoning behind this choice is that the product $\Delta_\Gamma g \Delta_\Gamma u$ is cancelled out, hence only products with at most two derivatives remain. We can integrate by parts to produce product terms with no derivatives or first order derivatives applied to each of u and g, so that $t(\cdot,\cdot)$ is a bounded bilinear operator on $H^1(\Gamma) \times H^1(\Gamma)$. The significance is we can then use this bilinear form in our finite element method which uses P^1 finite elements and hence is only H^1-conforming. The calculation is carried out below.

Lemma D.1.5. *Integrating by parts on* (D.3) *we obtain*

$$\begin{aligned} t(u,g) = \int_\Gamma \nabla_\Gamma g \cdot \left(\left[\frac{3}{2}H^2 - 2|\mathcal{H}|^2 - 2\right]\mathbb{1} - 2H\mathcal{H}\right)\nabla_\Gamma u \\ + \left(-\frac{3}{2}H^2|\mathcal{H}|^2 + 2\nabla_\Gamma\nabla_\Gamma H : \mathcal{H} + |\nabla_\Gamma H|^2 + 2HTr(\mathcal{H}^3) + \Delta_\Gamma|\mathcal{H}|^2 + |\mathcal{H}|^4 - 1\right) gu \, do. \end{aligned}$$

Proof. To prove the assertion we will work on each line of the expression for $t(g,u)$

in turn. First notice

$$
\begin{aligned}
&\int_\Gamma (\Delta_\Gamma g + |\mathcal{H}|^2 g)(\Delta_\Gamma u + |\mathcal{H}|^2 u) - (-\Delta_\Gamma g + g)(-\Delta_\Gamma u + u)\, do \\
&= \int_\Gamma (|\mathcal{H}|^2 + 1)(\Delta_\Gamma (gu) - 2\nabla_\Gamma g \cdot \nabla_\Gamma u) + (|\mathcal{H}|^4 - 1) gu\, do \\
&= \int_\Gamma -2(|\mathcal{H}|^2 + 1)\nabla_\Gamma g \cdot \nabla_\Gamma u + (\Delta_\Gamma |\mathcal{H}|^2 + |\mathcal{H}|^4 - 1) gu\, do.
\end{aligned} \tag{D.4}
$$

For the next line observe that

$$
\int_\Gamma 2H\mathcal{H} : (g\nabla_\Gamma \nabla_\Gamma u + u \nabla_\Gamma \nabla_\Gamma g)\, do = \int_\Gamma 2H\mathcal{H} : \nabla_\Gamma \nabla_\Gamma (gu) - 4H\mathcal{H}\nabla_\Gamma g \cdot \nabla_\Gamma u\, do.
$$

Furthermore, using [27, Theorem 2.10],

$$
\begin{aligned}
&\int_\Gamma H\mathcal{H} : \nabla_\Gamma \nabla_\Gamma (gu) = \int_\Gamma \sum_{\alpha,\beta=1}^{2} H\mathcal{H}_{\alpha\beta} \underline{D}_\alpha \underline{D}_\beta (gu)\, do \\
&= \int_\Gamma \sum_{\alpha,\beta=1}^{2} \underline{D}_\alpha \left(H\mathcal{H}_{\alpha\beta} \underline{D}_\alpha (gu)\right) - \underline{D}_\alpha (H\mathcal{H}_{\alpha\beta}) \underline{D}_\beta (gu)\, do \\
&= \int_\Gamma \sum_{\alpha,\beta=1}^{2} H^2 \nu_\alpha \mathcal{H}_{\alpha\beta} \underline{D}_\beta (gu) - \underline{D}_\beta \left[\underline{D}_\alpha (H\mathcal{H}_{\alpha\beta}) gu\right] + \underline{D}_\beta \underline{D}_\alpha (H\mathcal{H}_{\alpha\beta}) gu\, do \\
&= \int_\Gamma \sum_{\alpha,\beta=1}^{2} -H\nu_\beta \underline{D}_\alpha (H\mathcal{H}_{\alpha\beta}) gu + \underline{D}_\beta \underline{D}_\alpha (H\mathcal{H}_{\alpha\beta}) gu\, do \\
&= \int_\Gamma \left(\nabla_\Gamma \nabla_\Gamma H : \mathcal{H} + 2|\nabla_\Gamma H|^2 + H\Delta_\Gamma H\right) gu\, do.
\end{aligned}
$$

The final line follows by using the fact $\Delta_\Gamma \nu = -|\mathcal{H}|^2 \nu + \nabla_\Gamma H$ (see [22, Lemma 3.3]). We have thus shown

$$
\begin{aligned}
&\int_\Gamma 2H\mathcal{H} : (g\nabla_\Gamma \nabla_\Gamma u + u\nabla_\Gamma \nabla_\Gamma g)\, do \\
&= \int_\Gamma -4H\mathcal{H}\nabla_\Gamma g \cdot \nabla_\Gamma u + 2\left(\nabla_\Gamma \nabla_\Gamma H : \mathcal{H} + 2|\nabla_\Gamma H|^2 + H\Delta_\Gamma H\right) gu\, do.
\end{aligned} \tag{D.5}
$$

Continuing with the main calculation, now consider

$$\begin{aligned}\int_\Gamma -\frac{3}{2}H^2(g\Delta_\Gamma u + u\Delta_\Gamma g) &= \int_\Gamma -\frac{3}{2}H^2\Delta_\Gamma(gu) + 3H^2\nabla_\Gamma g\cdot\nabla_\Gamma u\, do\\ &= \int_\Gamma -\frac{3}{2}\Delta_\Gamma(H^2)gu + 3H^2\nabla_\Gamma g\cdot\nabla_\Gamma u\, do\\ &= \int_\Gamma -3(H\Delta_\Gamma H + |\nabla_\Gamma H|^2)gu + 3H^2\nabla_\Gamma g\cdot\nabla_\Gamma u\, do.\end{aligned} \tag{D.6}$$

Combining equations (D.3) through to (D.6) we obtain

$$\begin{aligned}t(u,g) = &\int_\Gamma \nabla_\Gamma g\cdot\left(\left[\frac{3}{2}H^2 - 2|\mathcal{H}|^2 - 2\right]\mathbb{1} - 2H\mathcal{H}\right)\nabla_\Gamma u\\ &+\left(-\frac{5}{2}H^2|\mathcal{H}|^2 + 2\nabla_\Gamma\nabla_\Gamma H : \mathcal{H} + |\nabla_\Gamma H|^2 + 2HTr(\mathcal{H}^3) + \Delta_\Gamma|\mathcal{H}|^2 + |\mathcal{H}|^4 - 1\right)gu\\ &+\left(\frac{1}{2}H^4 - H\Delta_\Gamma H\right)gu\, do.\end{aligned}$$

As we are considering a Willmore surface the mean curvature H satisfies

$$\frac{1}{2}H^3 - \Delta_\Gamma H = H|\mathcal{H}|^2,$$

hence

$$\frac{1}{2}H^4 - H\Delta_\Gamma H = H^2|\mathcal{H}|^2.$$

Inserting this into the equation for $t(u,g)$ above completes the result. □

Derivation of the second variation of the area and volume functionals

We also require the first and second variation of the area and volume functionals, which are

$$A(\Gamma) := \int_\Gamma 1\, do \quad \text{and} \quad V(\Gamma) = \frac{1}{n+1}\int_\Gamma id_\Gamma\cdot\nu\, do.$$

Corollary D.1.3. *The first and second variation of the area functional $A(\Gamma)$ are given by*

$$\begin{aligned}A'(\Gamma)[u\nu] &= \int_\Gamma uH\, do,\\ A''(\Gamma)[u\nu, g\nu] &= \int_\Gamma ugH^2 - u(\Delta_\Gamma g + |\mathcal{H}|^2 g)\, do.\end{aligned}$$

Proof. The transport formula (4.3) directly gives the first variation. The second variation is then obtained from Corollary D.1.1. $\square$

Using integration by parts, we obtain

$$A''(\Gamma)[u\nu, g\nu] = \int_\Gamma \nabla_\Gamma u \cdot \nabla_\Gamma g + (H^2 - |\mathcal{H}|^2)ug \, do.$$

Corollary D.1.4. *The first and second variation of the volume functional $V(\Gamma)$ is given by*

$$\begin{aligned}
V'(\Gamma)[u\nu] &= \frac{1}{n+1} \int_\Gamma u - id_\Gamma \cdot \nabla_\Gamma u + id_\Gamma \cdot \nu u H \, do, \\
V''(\Gamma)[u\nu, g\nu] &= \frac{1}{n+1} \int_\Gamma g\mathcal{H}\nabla_\Gamma u \cdot id_\Gamma - id_\Gamma \cdot \nu(\nabla_\Gamma u \cdot \nabla_\Gamma g + u\Delta_\Gamma g) \\
&\quad - H id_\Gamma \cdot (u\nabla_\Gamma g + g\nabla_\Gamma u) + \big(2H - id_\Gamma \cdot \nu|\mathcal{H}|^2 + H^2 id_\Gamma \cdot \nu\big) \, gu \, do.
\end{aligned}$$

Proof. The transport formula (4.3) directly gives the first variation. The second variation is then obtained from Corollary D.1.1 and Lemma D.1.3. $\square$

Using integration by parts, we obtain

$$\begin{aligned}
V'(\Gamma)[u\nu] &= \int_\Gamma u \, do, \\
V''(\Gamma)[u\nu, g\nu] &= \int_\Gamma Hgu \, do.
\end{aligned}$$

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